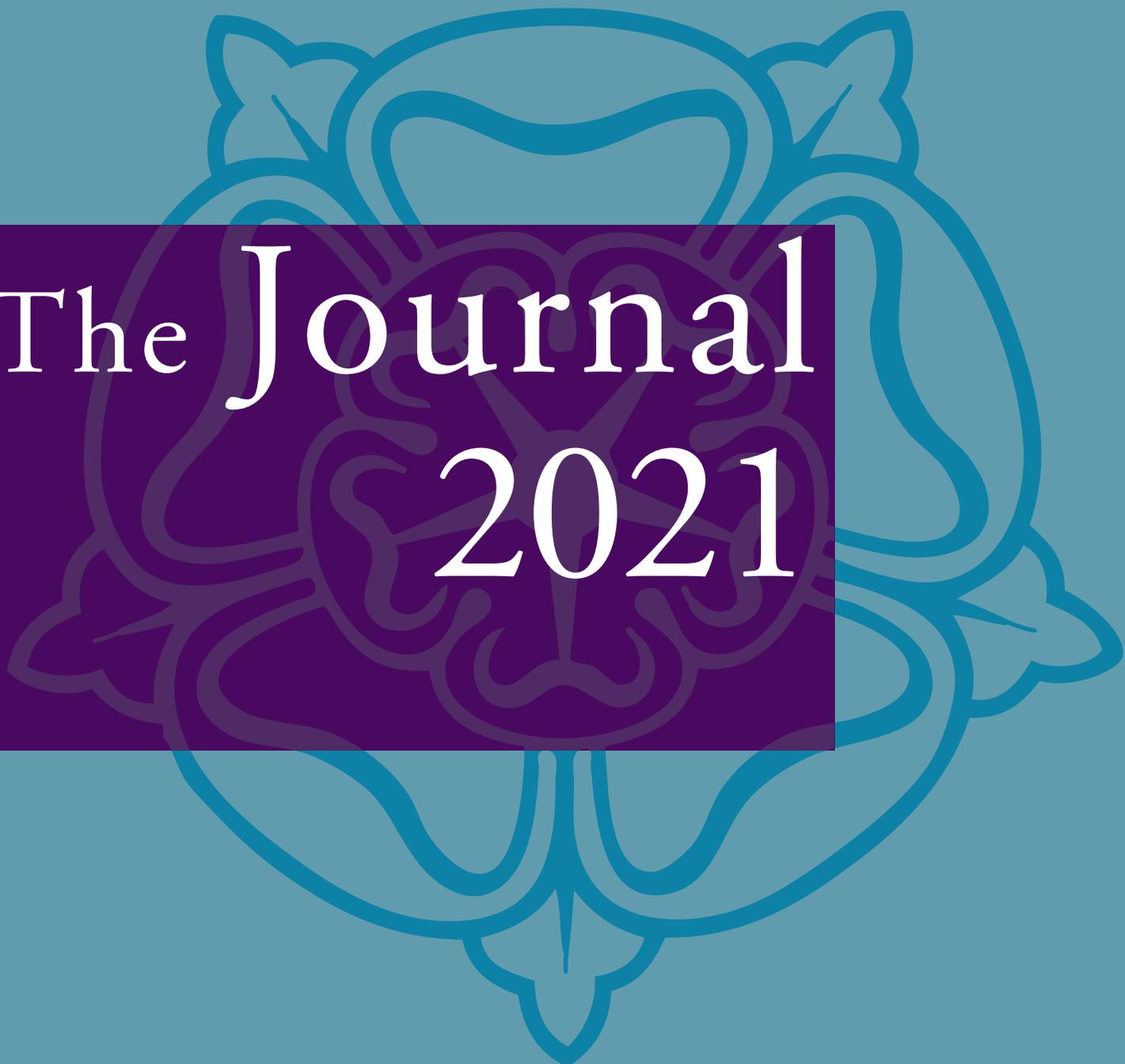




The Journal
2021



*'The world of reality has its limits;
the world of imagination is boundless.'*

Jean-Jacques Rousseau



From the Headmaster

The maxim – *Be stubborn about your goals, flexible about your methods* – has never felt more apt and could so easily sum up the culture of teaching and learning at the RGS over the last twelve months or so. Our whole community remains staunchly united in our goals: a love of learning for its own sake; a willingness to challenge and question; a desire to take pride in each and every part of our performance; a thirst for self-improvement; and so I could go on.

The days where education was delivered in a didactic manner from the front of a classroom to row upon row of passive learners is, thankfully, an anathema of the past. The pandemic has forced teachers and students alike to be innovative and flexible in terms of how they realise their targets. Flexibility and creativity are inevitably values which will have increasing prominence in the world in which we live and if the articles in this edition of *The Journal* are anything to go by, then the future is extremely bright. Once again, it is not only the sheer maturity, complexity of thought and conviction of these submissions which impress; equally, it is the genuine excitement, enthusiasm and passion which shine through each and every piece of work. Our students, having had a seed of inspiration sown, have put into practice all those elements of scholarship which allow quite exceptional results to be realised.

I would like to take this opportunity to congratulate my Head of Scholarship, Mr Bradford, and all those students who have contributed to *The Journal*. As this is Mr Bradford's final edition, I would also like to thank him for his astonishing work in this role, especially for nurturing such a collaborative, inspirational and exciting culture of scholarship at the RGS, and for initiating *The Journal* which is an extraordinary legacy, one which, I have no doubt, will continue for many years to come.

Dr Jon Cox
Headmaster



Editorial

Few years have required such perseverance as the last. A pivot to remote learning and the diminution of the normal collaborative manner in which students study required them to exhibit character in ways never asked of them before. Necessity is the mother of invention, that much has always been clear, and a global pandemic whilst challenging to some has been liberating to those individuals with a singular attitude to scholarship. It has freed their schedules and allowed for the uninterrupted pursuit of individual excellence. The products which are contained within this compendium are, quite honestly, without comparison.

They include an extraordinary assessment of British Indian voting behaviour which was later presented to the Conservative Friends of India, works expounding the uses of Brouwer's Fixed Point Theorem and the modern marvel that is Supramolecular Cages, a fascinating project on the alternative sounds of non-traditional Octaves and a shrewd and insightful analysis of the Gacha Mechanism; and that's only the half of it. I hope you find these works stimulating, insightful and exemplars of our school value of scholarship.

Students of this school have a unique collective spirit, the definition of which I've always struggled to articulate. It is something of a melting pot of competition, cooperation and humility.

From the moment I became Head of Scholarship this is something I've strived to stoke the fire of. It is what makes this school special and it burns fiercely in each of our students. This year, more than most, the warmth of its glow has been felt across our community. We've pulled together, spurred each other on, and met this challenging time with both kindness and endeavour.

It has been the utmost privilege to serve this school and its students as Head of Scholarship. I am supremely confident my successor, Mr Herman-Wilson, will take up custodianship of this torch and keep it burning brightly, if not a little brighter still.



Mr CS Bradford
Head of Scholarship



Foreword

The RGS has always prided itself upon its ability to uphold and spur academic excellence. Sadly, too often, education conflates scholarship with exam success rather than what is far more important: the development of academic interest and insight. Perhaps, it is because of this that the Independent Learning Assignment is so special and held with such great esteem at the RGS. The ILA is the opportunity that all students have to undertake an extended project delving into the fields of academia that interest them, that exist outside the scope of any GCSE or A-Level curriculum. It is the opportunity given to go above and beyond what is usually expected of them, to challenge themselves academically, and to champion their own interests under the wing of an overseeing teacher.

What follows in this journal is an exploration into ten of the top ILAs from this year: an opportunity to see the pinnacle of academic achievement that an RGS student can acquire when given free reign. The spectrum of different titles explored provides insight into the academic diversity that is present at the RGS. The projects in this publication span from Supramolecular Chemistry, to a Sortition Government in the UK, to battery-powered jet engines. And indeed, these are just ten subjectively chosen from 150. All the other projects throughout the year were also highly commendable.

I would also like to take the time to thank Mr Bradford for running the ILA scheme. On behalf of the Upper Sixth Form and the finalists, I hope you enjoy reading the projects in *The Journal* as much as the authors enjoyed writing them.

Ben Watkins

Chair of the Senior Scholars' Council 2020



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Brown and Blue: An assessment of British Indian voting behaviour

Omeeta Atara

PREFACE

This paper explores the changes which have taken place to British Indian Voting behaviour over the past decade. British Indians and the changes to their voting behaviour are explored in-depth whilst considering a variety of key factors. These include economics, societal evolution, historical experience and religious teachings. Each factor is unique and has a distinct influence on how British Indians vote. However, most significantly they all combine to create the British Indian identity. The study uses Harrow East as an example of where specific changes have taken place. Whilst it is a local example, it holds relevance on a national scale. It is also crucial to show examples and evidence of electoral changes. Factors are also explained in the context of party policy. Specifically, how parties, directly or indirectly, have adapted the policies to fit the requirements of the British Indian population. The impact of the generational divide is also referenced within the context of historical immigration. As a result, it gives recommendations on how political parties can further engage with British Indians.

This project was inspired by my own political identity. I am a second-generation British Indian and actively campaign for the Conservative Party. The purpose of my project is to explore how my culture and political identity are related. Elections are the evidence of change, but this project explores sociological, historical and political entities. These combine to answer the question of why British Indians have changed in their voting behaviour. Further to this, I wanted to identify my own political factors that drive my decision-making process.

The project aims to show why British Indians are a crucial minority for elections and how complex they are. By presenting what motivates a British Indian's political choices it will also educate on how to win the vote of a British Indian.

INTRODUCTION

Behind the turbulence of the most surprising and unstable political decade ever there was a fundamental psephology change taking place. British Indians are the most populous and significant ethnic minority in Britain¹ and play a major role in defining our unique society. There are 1,451,862 British Indians² all of whom have their own unique story. Whilst British Indians are a limited percentage of the whole population they are concentrated in certain areas. This concentration means that in many urban constituencies they are a high percentage of voters. Individual constituencies are most affected by British Indians. British Indians have emigrated at different times, from different regions around the world and have different experiences; however, these experiences often define an individual's political identity.

I am a British Indian and seeing the changes which have taken to place within my community have inspired me to explore our political identities. My father, mother, uncles, aunts and grandparents have all shown changing political opinion and thoughts. These changes are important to my family but also important in British politics. Politics in the United Kingdom will be affected by these changes. The voting behaviour of this populous minority has changed rapidly with a swing from the Labour Party towards a modern Conservative Party. However, the pervading question is why have these changes occurred?

Before embarking upon a forensic look at why we have seen voting behaviour change, it is vital to define some key ideas and terminology. A British Indian is a citizen of the United Kingdom who has significant Indian heritage. This heritage is incredibly diverse, with British Indians having emigrated over the past 400 years. This inevitably leads to different experiences of Britain and politics; voting behaviour is also affected by an individual's experiences of political, social, cultural and economic life in Britain. However, there are often misconceptions that British Indians are all Hindu. Only 44% of the British Indian population are practicing Hindus. Hence it is important to acknowledge that any surveys or references to British Hindus may refer to a minority of British Indians. The other 56% have a significant proportion of Sikhs and Muslims who generally come from specific regions within India. British Indian is a diverse and widespread term for a variety of different cultural, religious and political groups which cannot be taken as a single block vote. Individuals in this ethnic minority have all evolved differently; it is vital to understand that environmental factors are crucial when considering voting behaviour. Understandably, British Indians all have differing environmental factors and hence vote differently.

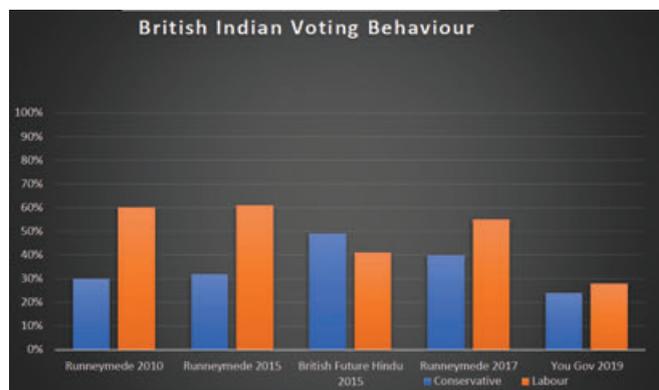
Ethnic minorities have generally favoured the Labour Party throughout electoral history. Labour recently claimed 77% of the ethnic minority vote in 2017³. Hence this has been an area in which Labour has relied upon. Labour internally and externally have faced criticisms for taking the ethnic minority vote for granted. They have shown a distinct lack of sensitivity when considering how policies will affect the ethnic minority communities. Often their specific policies have lost them support across all ethnic minorities. Chuka Umunna, a former Labour, Change UK and Liberal Democrat MP, accused his party of taking the vote "for granted."⁴ This stark acknowledgement of the party failing to understand the interests and requirements of these voters is a damning account of their behaviour. It is also important to acknowledge the failure of the Labour Party to promote ethnic minority candidates especially Indians. They chose no British Indian candidates for any key swing seats in 2019. Representation for British Indians across the Labour Party is limited; expanding this will help draw in voters. This failure to recognise the minority on a parliamentary level and a policy level is a disappointing failure. However generally, the Conservative party have



made efforts with ethnic minorities. Whilst they are haunted by the racist history of Enoch Powell, who gave the infamous Rivers of Blood speech, they have shed this image by engagement with ethnic minorities. The importance of this cannot be understated; put simply no ethnic minority voter will vote for a party linked to open racism.

Before embarking upon the reasons why we have voting behaviour change it is important to provide evidence to exemplify the changes taking place. Whilst polling specifically for British Indians is severely limited there are a few examples of polls which have been focused on British Indians and Hindus. The primary source is the Runnymede Trust which specialise in examining the electoral behaviour of ethnic minorities during elections. They acknowledged in their report on recent elections that there was a "noticeable change"⁵ in the voting behaviour of British Indians. Being the specialists in this area, they should be regarded as a trusted source of information. They show a significant narrowing of the gap between the Conservative Party and the Labour. The Conservative Party won 30% of the British Indian vote in 2010, a significant increase, however they won 40% in 2017. This is an increase of 140,000 votes. Increasingly, this has contributed to the significant improvement for the Conservative Party in the British Indian majority seats. These seats include Harrow East (used as a case study), Harrow West, Hendon, Watford, Finchley, Leicester South, Leicester North, Leicester East and Brent Central. In all these seats British Indians have caused either the Labour incumbents to be unseated or have a decreased majority in the last decade. The Runnymede Trust also argues that this is an "increased trend,"⁶ within the British Indian electorate; put simply more British Indians are voting Conservative. Hence, whilst we do not have exact statistics for 2019, we can expect British Indians to generally favour the Conservatives. The Runnymede Trust also use the largest data groups out of all the companies undertaking polls. They used 2,000 respondents which is a large sample. This increases the degree of accuracy by reducing the margin of error. However, there have also been other significant polls. The most recent is the You Gov and Optimus poll in 2019⁷. This poll was commissioned by Optimus, an Indian company and they teamed up with YouGov. They recorded a gap of only 4% between the two major parties; however, they found that the support was at the lowest levels of any polls. This is due to the "undecided" option which was placed. 18% chose this option and hence this support is likely to distribute between the major parties. Whilst it is the most recent poll and shows major declines to the Labour support and smaller declines to the Conservative support it is unlikely to be accurate. They only had 800 respondents which reduces the level of accuracy and is less representative. It is also widely accepted that the Conservative Party undertook a wide variety of new initiatives after this poll in November 2019. This is likely to have pushed more voters towards the Conservative Party. I will be referring to these initiatives later. The final poll to acknowledge is that of British Future in 2015⁸. Whilst this poll only surveyed British Hindu's who, as I alluded to earlier, are only a small proportion of British Indians, it does provide useful insight. It shows an 8-point lead for the Conservatives amongst the British Hindus. This is significant as it is the only poll which shows a section of British Indians having a clear lead and could be evidence of the religious diversions within the British Indian community. Furthermore, a poll by the same company of British Sikhs, many of whom are British Indians as well, came out with a lead of 8% for the Conservatives again (despite being a small sample). Whilst the British Hindu poll is more significant

as it was a large sample size of over 700 Hindus it shows that the two major ethnic religious groups are tending to the Conservatives. In conclusion, regardless of which poll you prefer or choose to believe the trend is that British Indians are voting more for the Conservatives. Whilst we can accept this the more interesting research is to find out why. Ultimately it is for a variety of political, social, economic, cultural and historical reasons which will not only shape the past but also the future of British society. However, this section demonstrates the stark changes which have taken place.



HISTORY OF BRITISH INDIAN IMMIGRATION:

Indians from all around the world have emigrated to Britain during the past 500 years; this emigration has occurred ever since the British set foot in India. Colonialism brought legal and cultural rights to Indians. At the time, these rights were a revolutionary idea; that the "savage world," could be attributed as British. The meaning of being an Indian changed with the actions of the East Indian Company and later the British Monarchy and Government. This section will show the diversity, value, and understanding that British Indians brought to this country and how their experiences have shaped their unparalleled political identity. It is vital to acknowledge the history of immigration. It is a history which at points has been turbulent, difficult, and traumatic. Much of the immigration has affected the British Indian voting behaviour today; especially that of the older generation. It will also show the wider integration and challenges faced by the modern British Indian community.

The East Indian company kicked off immigration to Britain through its requirement to have "lascars." These are men from the subcontinent who replaced British crewmen who passed away on the journey. Ultimately, they are Indian sailors who were picked up and brought over to Britain. Generally, the men came from the vital port cities of Goa and Bombay. Being South Indians, they had very different lifestyles to those of the North; they at the time were better suited to the industrial and naval lifestyle of Britain. The skills they picked up from the hustling ports in the area were easily transferred over to Britain. However, on the other side were the Indian servants who were brought back with their wealthy owners. They included nannies, cooks, and gardeners. These wealthy families who went out to the new subcontinent and wanted the continuity for their children but also the undeniably delicious food only the cooks from India could make. However, there is unsurprisingly a list of horror stories; British soldiers committed atrocities like rape, murder, and sexual assault. Often, there was a child born out of those horrors who was sent back to Britain to live as a mixed-race child. Whilst



regularly they were told they were not Indian and forced to hide it, there was the occasional success story, such as an individual setting up an Indian home here in Britain. Many children also came from marriages, soldiers had with women from the subcontinent and sent children and wives back to England. These were the original Indians living in Britain sometimes by force sometimes, by choice. Many of the families today can credit these amazing men and women with their origin. However, politically they were never involved as voting at the time was severely limited and hence, they never got the political opportunities. Many also lost their Indian identity with children, grandchildren, and great-grandchildren marrying British partners due to the lack of Indians in the country. Many lost their heritage and it is now estimated thousands of Britain's are unaware of this heritage. One of the key reasons why these sailors were required to settle down was the Navigation Act of 1660. It restricted the number of non-English sailors when traveling as a crew, and hence many Indians were required to stay, live, and settle in Britain.

However, another significant factor during this period was the scholarly immigration. The first recorded scholar of Indian origin to make the journey was: I'tisam-ud-din. He was a Bengali Muslim who in 1765 made the journey to Europe as a cleric, diplomat, and employee of the East Indian company. He famously wrote the Treaty of Allahabad. He returned to Asia after three years of living in Europe, as did many of the scholars at this time. The scholars took back culturally British Ideas to Indians but rarely laid down roots in Europe and established families.

In the 19th century, thousands of lascars, servants, and scholars came over to Britain in search of work and a better life. It is estimated 8,000 lascar sailors⁹ came over to Britain in this period. They lived and worked throughout Britain due to the East Indian Company and wealthy aristocratic families giving them the opportunity. Before World War II the Indian Congress conducted a survey and estimated there were 7,128 British Indians in 1931¹⁰. This is a number that rapidly increased after World War II. Ultimately the conclusion on the immigrants who came to Britain post-WWI is that they have often integrated into British Culture and statistics. Boris Johnson's great-grandfather was a Muslim who most likely came from India- yet he today is classed as a White British voter. Many of these immigrants are now in 6th and 7th generations in Britain and have hence lost their heritage. For those who retain, it is a very small proportion and hence they are generally described as "Anglo-Indians." This is a term to describe someone whose prevailing heritage is British but does have some minor Indian routes. Normally these voters are classed as "White" under surveys and hence for this piece I will do the same.

It is also important to acknowledge another significant, but indirect migration caused by imperialism. The British were very active in Africa; especially in areas such as Uganda, Kenya, and Tanzania. Thousands of Indians were encouraged to travel to Africa to work and live there. These African Asians often ended up in Britain after some horrific events. Post-WW2 the major development in this period was the British Nationality Act 1948. Established under the governments of Clement Atlee it enabled 800,000 Commonwealth migrants to come, live and work in Britain visa-free. It was a historic step in acknowledging the remnants of the empire. It allowed these migrants to be citizens of the United Kingdom. Whilst being a historic act, it did not intend for there to be general mass migration. Selfishly, they wanted to fill the gaps in the NHS, textile industry, and manual labour industry. The first

instance of mass migration was in 1947 when partition took place in India. This was a bloody separation between Pakistan and India. It was the beginning truly of the Muslim and Hindu divide. Indians from throughout the country, but mainly Punjab, came over to Britain and settled in the Northern counties such as Lancashire and Yorkshire. In an interview I had with Lord M Desai he spoke in length about the nature of these immigrants. He stressed they were "factory workers, allocated council homes, and joined the working class." These immigrants are the core Indian Labour voters. As I will continue to stress, they joined the traditional workers party as they were manual workers when they came to Britain. They came and were part of generally lower and working classes. They did not become professional. Generally, they remained in the underprivileged north. What is also crucial to note about these immigrants in the 1950s is that they suffered greatly from racism. They suffered from riots such as those in Notting Hill in 1958 and were battle-hardened. This continued to push towards Labour who were more sympathetic to these workers. I also had the privilege of speaking to Cllr. Reena Ranger who, in an interview with me, stressed that many of these workers came "heavily unionised industry and hence inevitably affected experiences." Working in an unionised job they were exposed to Labour ideas and philosophy. They have passed this down through generations and hence this where Labour picks up many of the votes. The final important thing to note is the loyalty of this group to "the person who let them in." Clement Atlee and his Labour Government gave them safe passage and hence they vote for his party out of sheer loyalty. British Indians are proud to have had the opportunity to come to this country and work. Many of them could only dream of this so it has enabled them to flourish. In modern times these Indians often reside in Manchester, Birmingham, Leicester, and Derby. Indians generally are very urbanised with 97% of Indians living in urban¹¹ settings, hence it unsurprising to see this statistic. This has also contributed to the voting behaviour, as Labour famously control urban areas with them winning all the Birmingham seats, Derby seats, and Manchester seats in 2019. Leicester, for example, has 28% British Indians. The majority living there as they were the 1940s and 1950s immigrants and still vote Labour. Overall, this is the band that Labour find they can rely, unlike the later Indian immigrants who are more flexible voters.

There was a period of immigration in the early 1960s and these were generally specialised workers. Gujarati's from the Gujrat region came over to Britain to work in textile industries. These regional workers specialised with this kind of skill. Hence, they came over here to utilise those skills in the booming textiles market. They were generally based in Bolton, Blackburn, Manchester, and Lancaster. They again fitted in with the working-class motive described by Lord M Desai, and they retained themselves as a Labour's stronghold.

However, British Indian immigration is a complex beast with there being multiple waves. In the late 1960s and early 1970s, there were two repulsive acts in former colonies that violently removed all Asian Africans. The first of these was in Kenya, where Jomo Kenyatta began a policy of Africanisation in 1963. This involved forcing Asians to surrender British Citizenship and claim Kenyan Citizenship. However out of 180,000 British Asians fewer than 20,000¹² submitted these applications. Some Africans now began to turn on the Asians, brutally enforcing Africanisation. They would favour Black Africans for jobs and fire Asians. The Kenyan Immigration Act 1967 forced Asians to get work permits and they began to suffer as a community. At this point



they were still able to emigrate to Britain and they did rapidly. Kenyan Asians, like my grandparents raced to make it to Britain. Life at this time had become dangerous in Kenya. Jomo Kenyatta had begun to rapidly expand Africanisation and these Asians often suffered greatly. Kenyan Asians settled across the country, however many settled in the areas surrounding Heathrow Airport. This where they either flew into and hence it was natural to settle around here. It explains how areas like Hounslow, Brent, and Harrow have become so populous with Indians. However, whilst London was the central base, Manchester and Cardiff also saw high populations. These communities often spread out quite heavily; they maintained smaller familial units rather than whole communities. Kenyan Asians were generally professionals however often had to take lower-skilled jobs. The desire they had to prosper has seen this generation rise through the cracks and grow in society. They now often have higher-skilled jobs and are economically prosperous. There were limitations and difficulties on immigration during this period - the Commonwealth Immigration Act 1962 was introduced by the Conservative Party as a response to growing public pressure over mass migration. It said that employment vouchers would be required for entry - however it failed to regulate effectively. The lack of enforcement meant it was still relatively easy for Kenyan Asians to make it to Britain. The Commonwealth Immigrants Act of 1968 went further to restrict immigration however again failed to do so fully due to a lack of clarity on how to handle illegal immigrants. The Act passed Parliament in three days out of direct fear that these Kenyan Asians - all 200,000 - would enter Britain. Many had made it before the Act however it did prevent immigration from Kenya until 1971. This caused many Kenyan Asians to become apathetic to the Labour government at the time and suffer severely in Kenya. These experiences explain why this cross-section of British Indians generally moves towards voting Conservative especially those in the south. Those in the North are swing voters who vote on individual concerns. Ultimately this group of Kenyan Asians is our intermediaries between the early Labour Indians and the later East African Indians. They are swinging voters who generally determine where much of the British Indian vote goes.

However, the next and final significant wave of immigration was that of Ugandan Asians. Uganda was a former British colony which saw a violent dictator in Idi Amin spring up in 1971. He was torn by the idea Africans were being neglected for the more prosperous Asians at the time and felt that he, like Jomo Kenyatta, had to take on a policy of Africanization. This policy was incredibly brutal and began by physically taking possession of these Asians and often ended in rape or sexual assault. However, his Africanization policy was based under the pretext of economic rebalancing - Ugandan Asians were the most prosperous ethnic group and owned many large-scale businesses. On August 8th, 1972 Idi Amin issued a decree giving the 60,000 Asians 90 days to leave the country. This rapid explosion caused 30,000 British Asians with British citizenship to flee to Britain. The dangerous story of the route is told by Lord Dolar Popat in his book – *A British subject*¹³. He describes making it through four checkpoints in order to get to the airport, he was searched and had belongings stolen. This is the very real story for 30,000 Uganda Asians who made it to the country. These Ugandan Asians were aided by Ted Heath and the British governments who gave them safe passage out of Uganda by commissioning special planes. Then they worked hard to find areas like Harrow, Hounslow, Hendon, and Southall for them reside and gave them jobs and protections. These Ugandan Asians have been

supported by the Conservative party on every step of their journey and hence many of them hold these loyalties true today. They also began in jobs that were lower paid but the desire to reach the standard of living which they had in Uganda encouraged them further. They had been the wealthiest society in Uganda and have tried to replicate this in the United Kingdom. Their skills as business owners and entrepreneurs shone through as they rose through British society.

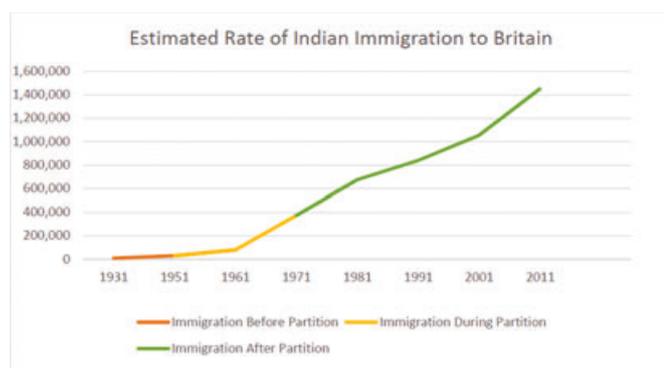
During this time there were also large numbers of illegal immigrants and undocumented immigrants. Throughout the late 60s and early 70s, those from Africa who were unable to come into Britain under the 1968 Commonwealth Immigration Act often tried to enter anyway. This was due to the limited provisions for deporting illegal immigrants. One such person who tried this is my maternal grandfather. In 1970 he travelled from Uganda to Britain amid fears Uganda would not provide the best home for his family. Whilst he came with seven friends and was detained illegally, his wife and two children headed to Kenya to be with family. He was at first detained at Harmondsworth Immigration Centre after landing at Heathrow Airport. After a process of interview and application, he was finally given the right to stay in the United Kingdom under the Conservative Government. He and his group of friends split up, some remained in London, others like my uncle went to Cardiff but he went to Manchester as he had wider relations there. For a year he grafted at manual labour and finally in 1971 he was able to legally bring his wife and kids. This is a true story and provides an example of the torture these families went through. As his grandchild, I am proud of his history and respect the suffering he went through to get his family the better life they deserved. Politically, he has always respected the idea the conservatives gave him the chance to enter Britain. However inevitably Enoch Powell and other influences have come into play and hindered his vote. How could he justify voting for a party which was openly racist...?

So, the story of the Ugandan and Kenyan immigrants comes together to give us the African Asians of the 60s and 70s who have integrated into our society. They are now the generally more Conservative voting because of who provided the opportunities. It is also important to acknowledge that the voters I describe here are the older generation - those grandfathers and grandmothers who now vote and live in Britain. They still remember these ties and base loyalties accordingly. Hence it is justified that these older voters of their generation see the wholly important factor in voting as the history. Therefore, the next conclusion to make is that it is virtually impossible to change these voter preferences. You can't change history simply and this is what matters to these voters.

¹⁴The next phase in British Indian immigration is in more recent times - those who have come to Britain in the past 30 or 40 years. Here has been no such "flood" of Asian migration at one sustained time but individuals or groups joining their families. One such was my dad, who came to Britain in 1983 as a 10-year old boy without his parents. He joined his uncles and aunts from Tanzania where his family moved to escape the terror of Idi Amin. His parents were unable to come but they wanted a better future and education for their children. Education is an important theme amongst British Indians and one I will refer to later. He experienced Britain during the Thatcherite Era of aspiration; this influenced his future as he tried to set up a better life for his family. I am proud of the links between my party and my heritage; it strongly supports my personal conservative belief in meritocracy and aspiration. Aspiration is a key theme throughout British India history and has



inevitably influenced political choice. Many of this generation to come are now still working with children and many are professionals. Whilst my father, a Gujarati Indian, works in finance, many modern dentists are Gujarati's and have been encouraged down this path. Hence, they are professionals, earning good money. They are politically very much swinging voters who look at the parties based on merits. Whilst history is important to them, they examine the facts which policies benefit them, which parties align with them, and most importantly where will they get the best result. British Indian population figures have been growing in the past two decades. However, this is more significant down to the generation now having children rather than immigration. These 2nd and 3rd generation Indians like myself will politically decide for themselves. They might have influences from lifestyle and status but primarily base decisions upon their experiences.



Indian immigration to Britain has an overarching effect on voting behaviour and is simply down to the generational change. Generally, those immigrants who came before independence have integrated so effectively into British Culture, they do not appear statistically Indian. On the graph on the next page they are represented by the red line and hence represent a small percentage of the total ever Indian immigration into Britain. Hence, for the purposes of this project are not part of the voting behaviour I have explored.

However, there is some immigration that occurred during the partition years which has affected British Indian voting behaviour significantly. The line graph below which is highlighted in yellow shows the immigrants from India who have begun to settle and work out lives. Hence, they can be counted as British Indians statically. Their heritage has pushed them towards voting Labour through the work of Clement Attlee. However, it is only those directly affected by allowance into the country who are truly guided by this. Children and grandchildren in some instances have moved away from the Labour Party in recent elections. Labour, however, have secured the older Indian vote as part of this generation. Their actions over the partition and the value of unionised jobs has won them the older voter but not the younger in Indian vote. It is also important to remember the majority of British Indians are younger (younger British Indians are also more likely to be politically active) and hence they have more significant electoral effects.

Finally, there are the East African and later migrants. They are shown by the green line and are the most significant group out of all the migrants. They are over 70% of the total Indian Immigration¹⁵ and hence are the significant part of the voters. The elder generation who immediately managed to make it to Britain during the reigns of terror in Africa must thank Ted Heath and the Conservatives for allowing them in and hence are loyal to that party. However, the actions of Enoch Powell did reduce

this loyalty by simple logic. As an outright racist in the Conservative Party he was unlikely draw in ethnic minority votes. On the other hand, anyone who is second, third, fourth generations have generally gained independence from this historical voting tendency. They vote based on other factors that I will further explore in this project. Indian Immigration is something which Britain should be proud of- we have allowed a new community to foster into British culture and politics. They play a significant part in our multicultural and diverse democracy. As an influence they are begun to grow economically and politically; this will continue to be explored throughout the project.

CASE STUDY: HARROW EAST

Harrow East is a constituency based in North London which is a prime example of where the Conservatives have won the British Indian vote. As a constituency Harrow East was formed in 1945, due to the boundary changes of Hendon and Harrow which combined to create this seat. It is important to acknowledge this seat is linked with Harrow West and they both are linked to Harrow Borough Council. It is a seat with a heavy British Indian population. As you can see from the table below, 6 out of 9 wards have a majority British Indians population with an average percentage of 40.42% and a total number of 35,137 British Indians. Hence it is a prime example to show what has happened at a local council level but also the general change on a national level.

Ward Area	Number of British Indians ¹⁶	Percentage of Local Population	Majority of British Indians	Number of Conservative Councillors
Belmont	5,292	46.65%	YES	3
Cannons	4,354	34.91%	NO	3
Harrow Weald	3,548	31.19%	NO	3
Kenton East	6,755	60.65%	YES	2
Kenton West	6,745	60.37%	YES	2
Queensbury	7,489	62.49%	YES	0
Stanmore Park	3,259	29.02%	NO	3
Wealdstone	4,420	38.79%	YES	0

What the census shows is that British Indians are the most prominent minority in the constituency, and they will inevitably shape the political landscape. Many have emigrated to Britain in the 1960s and 1970s and Harrow was a place where many settled. However, through relationships, we have seen children and second and third-generation Indians drive these numbers up. Hence this explains the earlier rise in the British Indian population.

On a local level, the council in Harrow is made up of Harrow East and Harrow West. The overall council is narrowly in favour of the Labour party overall however if you consider just Harrow East wards the Conservatives have 16/27 seats. However, whilst Labour holds the council by 35 to 28 in the specific Harrow East wards there is a Conservative majority; the Labour majority comes from Harrow West. However, on the local level, I have spoken to Cllr Ameet Jogia who is a Conservative in the Cannons Ward. He stressed that in the recent



byelection in the Kenton East Ward during April 2017, Nitesh Hirani (the Conservative candidate) gained the seat from Labour. He stressed the importance of this swing towards the Conservative Party and the fact there was a 19.5% swing. On a local level, this is an example of the major movement towards the Conservative party and representative of British Indians moving towards the Conservative Party. Kenton East is 60% British Indian and hence any swing is most likely to be based around this minority. Therefore, the evidence shows the radical changes in this swing constituency; these changes have been instigated by British Indian behaviour.

The council results show that in areas like Kenton East, Kenton West and Belmont all with Indian majority they have majority Conservative Councillors. Hence there is a correlation in this area between the number of Indians and the number of Conservative Councillors. Considering this council overall is Labour it is further evidence that British Indians in Harrow East have started voting Conservative overall.

Firstly, historically this has been a swing seat. From 1945 to 1950 they had a Labour MP, then until 1966, they voted as a majority Conservative. However, at this time it was a majority British constituency because as the earlier story told there had not been any migration at this time! Evidently then it does not reflect British Indian voting behaviour. In 1966 Labour won and then in 1970- 1997 it was a Conservative seat. However, during this period, it is important to acknowledge the British Indian population was still small. There had been many immigrants settling in Harrow after the waves from East Africa, but they were still the minority ethnic group. It is difficult to get exact results, as the first census results which can be relied upon are in 1991. Hence, we can only make educated guesses which have been done via immigration numbers. During this period, the methods for recording immigration were not effective. Therefore, we do not know the exact number of migrants during this period; most figures are estimates. However, the Indians were still outnumbered by the British electorate in Harrow East. So, despite the immigration they did not have significant electoral effects. However, in the future years, as these Indian families grew, they have taken however the constituency. Hence, in 1997 the seat turned Labour and in 2010 back to the Conservatives. The seat has interestingly followed the national trend and generally except for 1974, has been representative of the government.

It is also interesting to understand that the Labour MP between 1997 and 2010 was Tony McNulty. I was lucky enough to have some significant comments from him in which he described his actions in the constituency. He recalls his actions in understanding what mattered to the community. His actions have a set a precedent for good electoral practice in this community. In his comments to me he describes firstly getting involved in Navratri, Diwali and Aarti celebrations. His knowledge of local Hindu and Indian customs is impressive. By immersing himself within the community he does begin to gain the trust of British Indians. His understanding of their actions and mindset enables him to work with their holistic and social concerns. The immersion within the community and understanding of religious differences and significance is vital to his success as an MP. This is an idea I will touch on later in the report. He has done this further by understanding religious difference in the community. Lord Swaminarayan is a major differential within the wider Hindu movement. Some followers especially those with African backgrounds are very devout while other Hindus do not believe in this God. Tony McNulty acknowledges that in

his work he has showed sensitivity to these differences. The precedent of his actions includes setting up the Labour Friends of India who aim to rally the British Indian vote. He is a primary example of excellent electoral practice within the British Indian community. While an MP he also tried to understand the Pujaris. These are the religious leaders within Hinduism and have culturally sensitive roles. He understood and reacted to these as an MP. It is impressive to see the engagement with the local community and they do return the favour! He also sets the stage for the future interaction by Bob Blackman on a local level and David Cameron on a national level.

The significance of British Indians has been seen since 1997. They were the largest group in that period and voted in the Labour candidate. Thus, it changed to Bob Blackman MP in 2010. Therefore, British Indians as the consensus showed have driven towards the Conservative party in 2010. It is important to examine the results in the past four general elections.

Year of Election	Swing to the Conservatives
2010	+6.1%
2015	+5.7%
2017	-0.9%
2019	+5.0%

Except for 2017, there has always been a movement towards the Conservatives in the past 10 years and this is significantly down to British Indians. In an interview I had with Bob Blackman the local Conservative MP, he discussed the importance of the British Indian vote and the “incredibly hard” effort to gain these votes. He has valued the British Indian vote in winning him four consecutive elections in this constituency and puts a lot of the work by his British Indian community down to this. He describes his visits to Neasden temple and Diwali celebrations as a very important part of the engagement with the local community. It is important to acknowledge this as a local factor in swinging the vote in Harrow East. Many factors which Bob Blackman has exploited on a local level have been exploited on a national level by Theresa May, Boris Johnson and particularly David Cameron. So concludingly on a national level British Indians have voted for the Conservatives in recent years and switched from Labour. Excluding 2017, Bob Blackman has always increased his majority with a minimum of 5%. The British Indians have always been representative of the government of the day expect in 1974; which whilst holding limited value is an interesting representation of them. However, why on a local and national level has this change happened?

It is firstly important to say the national factors I intend to explore over the later course of this research do apply to do this local area. They have often been very parallel to many of the sociological, political and economic factors which have drawn the voters towards the conservative party. However, there are a couple of key things I want to mention which especially apply to Harrow East:

Firstly, is the action of Bob Blackman the local MP in Harrow East has made huge efforts to engage with the Hindu communities. Harrow East is around 35% Hindu population and Bob Blackman has made numerous efforts to engage with these voters. By hosting the Hindu Forum of Britain 2018 he showed real engagement and understanding



of integrating with the major electorate he faces. He worked and integrated with British Hindus to try and gain their votes; it is a very effective and clever tactic. By making this a public forum he learned and understood what was required and used this effectively locally and nationally. By learning the concerns, he created links that will become long term. However, it is not just this interaction in the forum but also the interaction at actual Diwali and temple-based events. As I mentioned earlier in his interview with me, he stressed the importance of this interaction with the community on their turf - he has been going to temples since the 1990s and this has been a clear local plan. He has actively engaged with his local community and deserves to represent them as their Member of Parliament.

There has been controversy over the Hindu events he hosted. In 2017 he hosted Tappan Gosh, an anti-Muslim nationalist. The Times heavily criticised him in an article critiquing Mr Gosh for supporting the Rohingya Genocide and Mr Blackman's insensitivity. There is no justification for the comments Mr Gosh made and opinions which are simply disgusting. I feel it was misjudged to invite him to somewhere as significant as the House of Commons. My support for Mr Blackman and the superb actions he has generally undertaken does not change - but it is right to condemn this mistake. However, the condemnation over the Hindu Forum where another Hindu nationalist who was notably much less controversial spoke is redundant. They were representing the governing party in India and those views - which are legitimate in India - must be heard.

Finally, the other important issue to discuss is Caste Politics. This issue is a hotly debated topic in Harrow East as a political controversy. Uma Kumaran has wildly accused Bob Blackman in the 2015 election of playing this game. He has been accused of pitting castes against each other. Further to this, he is accused of telling British Hindus the election was based around the caste system. Lord Dolar Popat has also been implicated by this and accused of using similar tracts. She has widely sanctioned this as "gutter politics,"¹⁷ She has referenced the leaflet to the left which shows the level of caste distribution. This leaflet was distributed by Mukesh Narkar, a Conservative Party member, and a believer in caste discrimination. She argued this was a direct order of

the Conservative party against her and others. She claimed the leaflet makes her fear the politics that was taking place in the area where she grew up.

Whilst any suggestions of caste politics are entirely unacceptable, and this leaflet is undeniably abhorrent. It is embarrassing that a Conservative Party member would do this. However, it is clear that this is not a directive from the party and not a directive from Mr Blackman. The suggestion from the Labour Party and Ms Kumaran is incorrect and unjustified. Cllr Ameet Jogia, in my interview with him, described it as "scaremongering." From interviewing and researching this issue I strongly believe it is not a genuine problem. I am a Hindu and have no interest in the caste system and neither does much of my family. It is not an issue parties should be engaging with, and it is morally wrong. Individual actions ought to be condemned but it is incorrect to assume that it is automatically from the party.

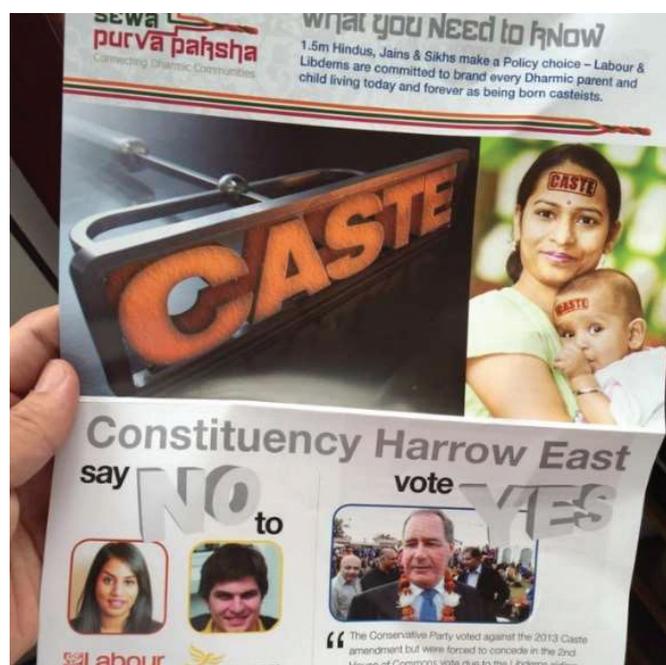
In conclusion, Harrow East is an amazing example of British Indians turning the elections towards the Conservative party. Bob Blackman has a lot to be thankful for as these minorities have pushed them towards a victory. They are the central reason for his success as the majority group in Harrow East. Hence it is a great example. There is also the basis for ideas that have been implemented nationwide to try and gain this vote. The Conservative group here have worked closely to address the British Indian concerns and issues and respected them. It is a great example of the changes we see on a national level which will be explored in more detail. This example of skilful electioneering should be acknowledged by all parties. Harrow East has been a fascinating constituency for those exploring the actions of this minority.

POLITICAL PARTIES

WHY NOT LABOUR

As well as considering why voters move towards the Conservative Party we also need to look at why the voters have moved away from the Labour Party. British Indians, as I established earlier, have generally voted Labour over the majority of their history. However, something has drawn them to the Conservative Party and equally importantly away from Labour. Hence, it is vital to realise both sides of the debate. Primarily, Labour has changed key policies in areas like Kashmir, religious matters, economics and education; all these issues are significant to the British Indian community. All of these issues have pushed away British Indians in the past 10 years all at different times. This section will focus on the direct mistakes of Labour regarding religious and ethnic conflict. Other party policy will be discussed when exploring the policies which matter to British Indians in later sections. Hence, this section will identify simply what the Labour Party has done wrong.

The first and most important issue is that of Kashmir. Kashmir is a volatile situation in a region of India and Pakistan which has never been stabilised. India and Pakistan both claim the whole of the region despite it currently being split. Whilst India generally runs the region, it is a Muslim majority region so many do feel it is unjust control. The Indian Government on the 23rd of September 2019 led by Narendra Modi, revoked Kashmir's special status to the shock of the international world. However, India refuses to acknowledge that it is an international issue along with many British Indians. It is important to remember this issue



is very significant to British Indians and Lord M Desai in his interview with me acknowledged this very strongly. Hence any developments on Kashmir can significantly affect how British Indians behave electorally.

The first significant development in the story of the Labour Party and Kashmir came in 2009 when David Miliband, foreign secretary under Gordon Brown, wrote an ill-informed article for the Guardian in which he discussed Kashmir. The fervent rule is that nobody should get involved in accordance with India's ideals. British Indians were inevitably disappointed when this interference occurred. In the prominent editorial, *The Hindu*, described it as an "ill-conceived foray."¹⁸ The Independent went even further to call it a "disaster."¹⁹ So immediately the mistake of Miliband, which he also made on his trip to India as foreign secretary, began the decline of the parties ill-fated policy.

Labour however, have always been active in the Kashmir issue as Lord M Desai acknowledged. As someone who was active at Labour Party Conference, he said that there were always "resolutions from constituencies, some pro-Pakistan, some Pro-Indian," submitted and then debated and a natural resolution proposed. It was a "minority issue." However in 2019 there was a significant yet alarming reaction.

The Kashmir Motion at the 2019 Labour Party Conference in Brighton was a significant area of frustration from British Indian voters when interacting with the Labour Party. As previously established, Kashmir is important to British Indians as many of them have strong feelings on the subject. Hence as this motion was implicitly in support of Pakistan it inevitably angered the British Indian community. The motion, which appeared on the Tuesday of the Conference, particularly angered British Indians with comments including "self-determination," and "international observers enter the region." Kashmir is a Muslim majority so India votes against self-determination as it would lead to Pakistan taking over. Many Indians also feel the historical balance belongs to India and hence they were frustrated to hear this. However, significantly the second part was the most frustrating. Kashmir is an internal dispute in the eyes of India, and hence sending in international observers would disagree with this - it implies it is an international issue. This has caused many British Indians to move away from the Labour Party and the electoral statistics back this up. However Lord M Desai disagreed with this - he argued that "it got more coverage in India than the UK." However, it may not have got mainstream media access in the UK but Indian communities have a "WhatsApp trend". Many families use WhatsApp as key communicating methods and socially spread messages on the platform. There was a widely shared message with this, proclaiming the Labour Party as pro-Pakistan. As this circulated through the families and communities many voters moved towards the Conservative party. WhatsApp messages are significant in other areas later. I believe this did affect the voting patterns and behaviours of British Indians despite Lord M Desai arguing otherwise. It is a significant factor. This was topped off by Jeremy Corbyn tweeting "The rights of Kashmiri People need to be respected." He again argued for self-determination and pushed Indians further away. I would also suggest here the official 2019 figures, when they are released, will clearly show British Indians being frustrated by this motion despite the desperate attempts of Ian Lavery. He sent British Indians a letter urging them to "not be alarmed," by this movement. However, Kashmir will continue to show movement away from the Labour party.

There are many consequences of this in the religious field which I acknowledged in my introduction to this section. Whilst they are the

same thing from a different angle they push Indians and the Labour Party away. Firstly, the Labour party can be seen as an "anti-Hindu" party. It is important to understand that this would be in direct opposition to the pro-Hindu government in India. Before continuing I will caveat this by saying that this applies to the 44% of Hindus who are British Hindus and practicing - evidently they will be significantly affected. The Hindu Council a significant body for British Indian Hindus and has openly called the Labour party under Jeremy Corbyn's "racist and anti-Hindu." Evidently, if I am a Hindu and have been told that the Labour Party is against my religion, to the point of being racist, I would not vote for them. Even more significant I would tell others not to vote for them and this is the basis and the WhatsApp messages which are sent out amongst the community. Hence, they do not just lose one vote from this but multiple - this is the ripple effect within the community. The significance of Anil Bhanot, the Director of the Hindu Council, cannot be understated. He is well respected in the Hindu community and was the "Hindu representative" at the wedding of the Duke and Duchess of Cambridge. He is regarded by Buckingham Palace and the Government as the authority within the Hindu community and hence his comments will be taken in the utmost seriousness.

There is lingering frustration over the partition mistakes made by Britain and India as a whole. Generally, Governments and parties have avoided the India and Pakistan to avoid offending the memories of partition. Labour are the first party in years to interfere in the relationship. This also frustrated many British Indians. Labour has also been accused of being Pro-Islamic and Pro-Pakistan. Whilst there is historical tension between Muslims and Hindus due to the atrocities which took place after partition, I believe that these in modern Britain have been pushed aside. In modern-day Britain, these tensions are at worst simmering below the surface but most likely to be non-existent. I do not condone the WhatsApp messages widely spread in Hindu communities which are Islamophobic. There is a more pressing issue of accusing Jeremy Corbyn, as leader of the Labour Party, taking them to a pro-Islamic standpoint. I don't believe this to be the case despite sites like the Spectator, Daily Mail and Sun all shouting about it. Jeremy Corbyn does not favour Islamists over other religions - he has regularly condemned examples of Muslim and Hindu mistakes. I am not a Corbynite by any means but these claims have no basis - his Kashmir stance, whilst not aiding his electoral cause to any degree is not on a religious basis. Hence, this should be dismissed as scaremongering and fake news.

It is also important to acknowledge the indirect effect of Anti-Semitism on ethnic minorities in general. Labour and especially Jeremy Corbyn have faced significant difficulties over anti-semitism over the past 5 years. It stems from the culture of the constituency parties and has infiltrated the wider systems and structures. For British Indians who have faced significant amounts of racism during their lives they have the ability to empathise with those who have also faced racism. The Jewish faith are undeniably uncomfortable within the Labour Party. British Indians are uncomfortable voting for a party which in anyway is perceived of slightly racist. Hence, they are less likely to vote for anti-semitic Labour Party.

In conclusion, when it comes to religion Labour has made serious mistakes with the British Indian community. The Kashmir motion shot themselves in the foot by supporting it so vividly. They have alienated the British Indian community. However, they have argued that it is the



same as the government stance. The government, however, do not call for an investigation, only peace and this is the vital difference. The interference inevitably caused disgust among British Indian Communities. However, to call Labour Po-Islamic is a step too far. This simply fails as there is no evidence. Anti-Hindu has a more plausible argument and something for Labour to address. Keir Starmer will need to resolve this and I will explore this in the area about solutions!

WHY CONSERVATIVE :

The Labour Party made some inherent mistakes in managing the relationships with British Indian voters and I acknowledged this in the earlier section. However, in the Conservative Party, there has been a concerted effort with ethnic minorities in general and particularly the British Indians. In the party, many senior figures have worked consistently to make this happen; this campaign has been lead by Lord Dolar Popat and David Cameron. They tried to modernise the Conservative Party with strategies and political campaigning with British Indians. However, they have also forged a stronger relationship with the popular BJP in India and an especially personal relationship with Narendra Modi. He is undoubtedly popular among many of the British Indians who appreciate his good work. Some British Indians do view India as "home" and hence the politics of India is very important to them. However, I would argue the most significant result of these actions taken by the leaders and activists across the country is that they have finally shed the Enoch Powell image.

The first key area to explore is the work of Lord Dolar Popat in modernising the Conservative Party structures and actions when interacting with British Indians. He came from Uganda in the 1970s whilst fleeing the brutality of Idi Amin as a teenager. He did what would now be "A-Levels" in Britain and worked at a wimpy bar. He came from humble roots in Britain and is an example of an excellent businessman. He owned a variety of businesses but specialised in care homes including the first-ever care home which was specially designed for Indians in Britain. My grandmother is now lucky enough to reside there. He joined the Conservative party in 1980 under Margret Thatcher. He says in his *Brown and Blue: An Assessment of British Indian Voting Behaviour* book that "winning Asian voters to the Tories, has always been a major focus for me."²⁰ Margret Thatcher as MP for Finchley had a constituency with a significant British Indian population and she met them in the summer of 1980 in a crowded town hall! It is this kind of engagement that sets out the future for the Conservative Party. Lord Dolar Popat was personally asked to try to build relations between the Conservatives and British Indians in the 1980s. Lord Dolar Popat in the 1980s worked for the Anglo-Indian Conservative Association to begin creating events for the community to rally around. This was popular but ultimately failed to win many more votes for the party. However, the greatest change to Lord Dolar Popat, as he says in his book, is "The Labour Party dedicated Taskforce to keep in touch with members of the Hindu Community,"²¹ and Gordon Brown beginning to send Diwali cards to the community. It is here that the story really changed and the Conservative Party began to finally effectively engage with these voters. Lord Dolar Popat having the realisation lead to so many of the amazing events which were hosted and I will begin to introduce. He genuinely changed the face of British Indians and the Conservative by engagement. He made an effort with the community in areas where many other leaders failed to inspire or even engage people. He

showed the community why David Cameron and the Conservatives were right for them.

The events which were held to show the engagement and the reasons why the Conservative Party was right for the British Community. However, I believe that British Indians felt embraced by the Conservative Party and the effort they were making. It is worth considering that British Indians by 2010 were becoming an even greater electoral force so it made logical sense for both parties to try and make an effort with them. The first events were small scale including David Cameron visiting Hare Krishna Temple in Hertsmere and then mentioned Diwali during PMQs. These minor but significant actions spurred the Conservative Party on to working even harder to engage British Indians across the country. However, when David Cameron gave a speech at a Hindu gathering in Leicester in this was the first major engagement. 5,000 British Hindus turned out to listen to him speak. It was a great moment for Cameron to begin to show British Indians why they should vote for him! However, this was all a plan worked up by Andrew Feldman (Conservative Party Chairman at the time) and Lord Dolar Popat to engage people. Engagement is the overriding strategy of this whole section and has proved a success electorally.

Since then the events came thick and fast, with the most significant being in 2009 when David Cameron held a Conservative Party Diwali Reception which drew in thousands of British Indians they saw there own culture replicated by another party and felt welcome and wanted. Cllr Ameet Jogia (an aide to Lord Popat) in an interview with me strongly acknowledged the value of this and the time Lord Dolar Popat had put into his work. British Indians are proud of both their British and Indian cultures but they are proudest when they see them merged like in this scenario. Theresa May spoke at the Hindu Forum of Britain to show voters why the Conservative Party might be best for them and this engagement was a vital part of the process.

The reason these British Indians voted for the Conservative Party in much improved numbers after 2012 is simply down to this work. British Indians felt like they were being directly helped and accounted for they were involved and accepted by the Conservative party. Generally, ethnic minorities need to feel welcomed within a party or the wider political scheme and this is what these actions achieved. The British Indians warmed to the efforts of the Conservative Party and ended up voting for them. I also think the skill of using urban locations such as London and Leicester should not be understated. Lord Dolar Popat stressed it as well- British Indians are generally in Urban locations and the report by policy exchange found the 97% of British Indians are urbanised²² and hence this was another effective strategy to target British Indians.

There has also been a continued effort since David Cameron established this trend of giving Diwali messages to the community. Theresa May did so in office but Boris Johnson gave a striking and impassioned message. He firstly, embraces the culture talking about "Lord Ram and Sita, the festival of light and Ravana." These are characters and ideas vital to British Indians, who felt the UK Prime Minister is truly understanding and engaging with the culture. It gave me a warm and proud feeling to hear it spoken by the Prime Minister. His effort to understand the culture is appreciated by British Indians. However, his message continued to be poignant and reflective. He also discusses the value and importance of British Indians to the United Kingdom. The contributions they make to "business, science and public



services," are applauded. These all make the community feel welcome, valued and proud. It unites the two different cultures and to see the PM embrace British Indians is a great feeling. However, the most proud moment is the comment " Britain would be a lesser country without your contribution." The conclusive remark is well placed, true and warming to British Indians. It was a superb message from Boris Johnson and something the British Indians truly appreciated. There was a superb community response to the video; it has become a great way to interact with minorities and in this example it resonated with the British Indians. In addition, this trend has set a good tone for British Indian and Conservative relationships.

Moving on Lord Dolar Popat and David Cameron established the CFI- Conservative Friends of India, of which I am now a member of and two people who I have interviewed- Cllr Reena Ranger and Cllr Ameet Jogia are co-chairmen. I have a great chance to get involved with Conservative Party Politics through this and I have been appointed a Regional Champion for my area by this group! Lord Dolar Popat set it up to link the Indian community, Indian Parliamentarians, and the Conservative Community. It was an exciting venture to continue this extremely important relationship. Cameron and Lord Popat continued the work by giving a speech to 1,200 key members and then a historic visit to Neasden Temple. This was a superb moment for this new group and showed the real and genuine impact they had. The CFI has held regular dinner and engagement events as well as policy forums that are fed directly back to the upper echelons of the party. It enables British Indians to have their voice heard through this mechanism and continues to draw people towards the Conservative party. It's work has definitely helped David Cameron gain a majority in the House of Commons in 2015. However, arguably the most significant part of the work as the song "Neela Hai Asman." It is song made specifically for the British Indian community. I was also somewhat shocked and confused as to why the party would do this, especially for Indian voters. It is a Hindi song meaning Blue Sky and was commissioned to encourage British Indians to vote David Cameron by directly engaging in their own language and culture. The video showed photos of David Cameron at temples and praying whilst also arguing policy points. British Indians had never had such engagement politically with them directly and the Hindi song hit a note with many in the community. It did not just resonate in the community but it went viral in the weeks leading the 2015 election. The British Indian community was engaged and proud of this song. It is a tradition in the party and something which the community adores.

Lord Dolar Popat is inspirational for the way he has led the Conservative Party into a new era with these voters. He ought to be praised undoubtedly for his work and skill in engaging the British Indians. His work has discovered how parties can work with the group effectively and both political parties should be taking note of this. These events have inevitably increased the vote share for the conservatives over the past decade. He has effectively worked with leadership to set up the CFI and left a lasting legacy. He is the greatest success of the Conservative Party for British Indians and his work has swung the voting towards the Conservatives.

The Conservative Party has also forged stronger relationships with India as a country. India is currently lead by Narendra Modi who was formerly governor of Gujrat a state where many British Indians, including my family, hail from. Firstly, David Cameron and his foreign secretaries William Hague and Phillip Hammond have worked very

hard to develop a relationship with India. India is currently lead by the Bharatiya Janata Party (BJP) and they have control of the Lok Sabha. The party itself is a broadchurch right wing-party with a strong Hindu nationalistic viewpoint. Hence, generally, they marry up well with the conservative party. In the book, *Indian Conservative* by Jaithirth Rao discusses the "synchronicity between Anglo Saxon and Indian Conservatism."²³ In reality, it is evident that Anglo-Saxon Conservatism has inspired the Indian Consitution after partition to an extent. Hence, it is natural that there is a good relationship between these nations. However, the relationship went a step further under David Cameron.

In 2014 David Cameron hosted Narendra Modi in Britain. His memoirs detail the value of this relationship but he implies that he was the only other foreign leader to get the same treatment as Obama. However, there was a significant event in which David Cameron served as a warm-up act for Narendra Modi. In 2015, Wembley Stadium was packed out with British Indians who all came out to hear the both of them speak. In this speech, David Cameron praised British Indians for the work they do for the country and the party. However, Narendra Modi spoke about the beauty of the relationship between the countries whilst under the Conservative Party. Inevitably British Indians want their home country and resident country to have a strong relationship; this is evident here! The event turned into a celebration of all things to do with British Indians and how they were central to the future. As I alluded to earlier British Indians loved the sense that their two identities were joining together under the Conservative Party. The event was widely shared in India and Britain and showed the relationship between the parties in policy and ideology. Narendra Modi is a hugely popular figure among British Indians for the work he has done in India and hence many do feel that a relationship with him would be good for them. Further to that there have also been visits by William Hague, Phillip Hammond, George Osborne, Priti Patel, Lord Dolar Popat, and David Cameron himself in an attempt to forge good trade relations. In fact, British Indian trade has improved and increased they are a big "post-Brexit partner." There have also been reports of free trade agreement between the countries which would further strengthen the relationships. Whilst debate will loom large it is unarguable that Britain and India have grown in friendship and hence British Indians and the Conservative party, who have lead this movement have grown even closer.

The final key idea which almost draws all of this together is the removal of the Enoch Powell imagery. It is astonishing to think his former party got one million ethnic minority voters in the 2015 general election. Enoch Powell is famed for his "Rivers of Blood Speech," which he made to the Conservative Party Centre in Birmingham. His ideas of "madness" for the "50,000 dependants," almost pushed all ethnic minorities, including the British Indians, over towards Labour. Logically, the British Indian and other ethnic minority community at the time were unlikely to remain in party where they suffer from racial abuse.

Despite Powell defecting to the Ulster Unionists 6 years after this speech, the Conservatives have never really managed to shed this notion of being the upper class and racist party. Lord M Desai was very firm in suggesting that "John Major, the working class Brixton boy," was vital in removing this image. The Conservative party did have the working class leader in the early to mid-90s with John Major as Lord M Desai correctly stated leading the party from a working-class background. Brixton is an area in London with large numbers of ethnic minorities however the



central basis for the population is the Caribbean. It is important in my opinion to acknowledge that this did a lot to refute the upper-class and posher image with the ethnic minorities who saw the Conservative Party negatively. However, I again disagree with the importance he places upon the value of John Major. Whilst he may have changed the image he did not manage to translate this to electoral success. In 1997 Blair achieved a huge win with the ethnic minorities, almost entirely voting Blair. From discussions with my family, I have found that they all voted for Blair and hence whilst John Major changed imagery he failed to truly translate it into electoral success. Further to this, I would also argue that that whilst the image was more reputable, the Conservatives were still seen as less friendly to ethnic minorities. As Theresa May acknowledged when she gave a speech as a Conservative party chairwoman they were the "nasty party."

Hence, Cameron has not just gained votes but been forced to change this aspect. He has used more friendly approaches with the public aiming to show the Conservatives are not nasty. He has been seen on his religious temple visits and making an effort with all ethnic minority groups. However, what is most important is that change in tone and rhetoric. Rather than being critical of reforms of Blair which were hugely popular- which leaders like Ian Duncan Smith and Michael Howard might have done- he focussed on critiquing reforms who were not popular. It sounds entirely logical but he played the "pragmatic Conservative" role. He was hard on the Iraq War and fiscal mistakes. The public did not see the party as nasty because Cameron spoke about the value of everyday life and the NHS. Shedding this image of nasty to being slightly more friendly has opened the ability to win electorally. He has changed the party for ethnic minority voters.

It is also important to understand that the Conservatives have been forced to undertake a cultural revolution within the party. To win Indian voters they need to make the party more accessible for

British Indians. Whilst Lord Dolar Popat is the traditional example there is another interesting story. Before he rose to prominence Shailesh Vara lead the charge by British Indians in the Conservative Party. He was a prominent Conservative Party member in the 1990s by leading Party Conference debates against significant members like David Cameron. He competed as the lead speaker on the debate in law and order whilst being one of very few BAME members at the time. The Conservative Party can be seen as backward with a distinct lack of BAME support. During the Black Lives Matter movement, they have come under intense scrutiny over this perceived lack of diversity. As a Conservative Party member, I can definitively say that there is no widespread racist issue within the Conservative Party. There are individuals who hold unacceptable views and they will be disciplined fully. However, they are not inherent racist now. Shailesh Vara tells a depressing story of how the Conservative Party has modernised its approach specifically to British Indians. In 1997 he stood in the constituency of Birmingham Ladywood which is a safe Labour seat. He was elected the Deputy Chairman of the Conservative Party after this. He inevitable was a senior figure within the party operations and clearly aimed to make it into Parliament. However, he was regularly faced with barriers because he was an immigrant, in an interview to me he described the depressive picture of being told he would never be getting a safe seat. In 2001 he was advising Michael Howard and the media spokesperson. He again was given the seat of Northampton South. As one of the most senior Conservatives who was not in

Parliament you would expect him to take a safe seat. He was bluntly not given one and forced to take a marginal. He lost by 85 votes. The inherent issue was that he was an ethnic minority and not seen as a safe part of the party. As Deputy Chairman you would not expect this to be the case. He eventually managed to almost singlehandedly change attitudes. His story which he told to me in an interview shows how the conservative party could not target British Indians externally without addressing the internal issue.

In conclusion, the concerted effort lead by the Conservative Party is very much noticeable. They have worked tirelessly to improve their standing with ethnic minority voters and used generally effective techniques. The direct engagement and image shedding is crucial in showing voters they can vote Conservative. The relationship with India formed out of policy, has been a great success. Whilst they have managed to gain electoral success it is interesting that arguably in 2015 there was the greatest swing. This implies the relationship with India might be the most valuable of all the factors. Events like the great Wembley stadium speech should be replicated because British Indians responded amazingly to it. I will discuss this more in the recommendations sections but for now, this is a huge path forward. Lord Dolar Popat is the main character for the party and his tireless work has been of great success to the party nationally and the key reason why they were able to return to Government.

OTHER FACTORS

ECONOMICS

As acknowledged earlier, the second and third generation Indians are overwhelmingly rational rather than emotional when it comes to picking a political party. They will consider the level of engagement of the party with the community, but primarily they will vote on self-interest. They will vote for the party which will best serve their interests sociologically, economically, culturally, and politically. The Conservatives have already been engaging with the community on a number of levels but this is not enough they need a policy to match up with the needs of the community. A significant area where this has happened is in the economic sector.

Indians have progressed economically over the past decade leading the charge in professional services especially business and law. Hence we have seen that Indians are wealthier than they were years ago. The statistics back this up- British Indians have the highest median wealth out of everyone at the country standing at £178,980²⁴ which obviously shows they are one of the wealthier groups in society. However, they also the most likely ethnic group to have weekly earnings of over £1,000²⁵. This shows they are the top end of the spectrum whilst also being the second least likely to earn below the minimum wage²⁶. They also have the second-lowest unemployment rate at 8%²⁷ with only White British having it lower at 5%. Hence British Indians are among the wealthiest and most privileged groups in our society.

Whilst I am by no means suggesting that just because they are wealthy they will vote Conservative, there is an undeniable electoral link. Conservatives generally tend to pick up the most votes in the "A and B" classes. British Indians came to this country as poor immigrants but have worked their way up the social classes. This is something I have seen my parents, my wider family, and Indian mentors such as Lord Dolar



Popat achieve. The changing circumstances are an explanation of why they have recently begun to vote Conservative and not historically done so.

Hence we need to address, why do the Conservatives appeal economically? I think the first answer is in the low tax policies. In the 2019 General Election, the Labour Party came out and gave rapid tax increases. Jeremy Corbyn in his manifesto, wanted to raise taxes on income (over £80,0000), VAT, and National Insurance. Inevitably, this would affect everyone but especially the higher earners and hence British Indians would not want to give away more money. They have worked hard for money do not want more taken- that is just simple logic. This is where party policy from the Labour Party has not reflected the interests of many British Indians. This is not to say all British Indians are rich and against high taxation but generally I would argue this is the case. Hence the Labour Party policy turned them away. Many British Indians also felt that the tax money taken would not be effectively used. On average each person would pay £2,400 more per year under Labour. This general feeling amongst the community hampered Jeremy Corbyn's bid for No10.

However, Boris Johnson and his Conservative Party came out on a completely different strand. He came out with a "Triple Tax Lock." This vowed to not raise Income Tax, National Insurance, and VAT in stark contrast with the Labour Party. Hence British Indians also were drawn into this policy. However, his rhetoric of the Conservatives being the "Party of Business", which again contrasted with Corbyn who focussed on workers and employees, was popular with British Indians. Many British Indians own businesses or work in high-level businesses and the promise to review business rates and at some point cut corporation tax were popular. Hence they would vote on what would directly affect them. Historically British Indians, when they emigrated, did set up wholesale businesses in East London and they have grown today. However I think culturally British Indians have the "entrepreneurial spirit," and to have this stymied by the Labour party would be frustrating. Especially the Ugandan Asians who were businessmen when they lived in Uganda. Hence the Conservatives economically have naturally had tax policy appeal for the British Indian community.

There is also more cultural economics to explore. In recent years the policy of austerity has been pushed through by George Osborne and David Cameron. Whilst a controversial policy across the country which has many critics it did appeal to British Indians. British Indians are not expansive monetarily they believe in saving not spending. This is not an economic but cultural decision. They are against short term high-interest loans and tend to save money. The common idea is – "staying within your means." They spend what they have and what they earn. This is not all British Indians but a common theme. Hence, they did buy into this idea on the wider economic scale. Austerity was sold about saving our deficit and slowing down borrowing which was something the British Indians bought into. My father and wider family have also been talking about the value of "saving," and as earlier acknowledged British Indians have the highest levels of savings. This frugal nature was linked to the Conservative policies and was another reason the voted with the Conservative's economic policy. In comparison to the Labour party where Gordon Brown and Ed Miliband wanted to spend excessively and borrow heavily. These Keynesian economics were rejected by the British Indians because they disliked the spending and risk which came with borrowing. Stimulus is a valid economic idea but it did not follow

the cultural British Indians. Whilst it is not the party's direct fault, it did not ring the right message with British Indians.

In conclusion, British Indians have managed to climb through the economic classes over the past few years. They have managed to earn higher wages and reduce poverty among the group. This drew them to the "natural party" of the rich which is the Conservative Party. Levels of taxations have been a huge issue for British Indians and the Conservative Party has won this debate. Finally the cultural attitude of "saving overspending," has been applied on a national level by the group. Hence the party policy has naturally been drawn to the Conservative policy and they have naturally gained this vote.

EDUCATION

Tony Blair's famous slogan of "Education, Education, Education," certainly rang true to the British Indian community. When Indian's emigrated to Britain 19% of immigrants came to be students²⁸ directly showing how greatly they valued the education system. However, a further 48% came for a better life which was largely based around the desire to provide a better education²⁹. The overriding reason Indians came to Britain is to give their children and families a better education and future. Hence in the years in which they have been here, there has been a concerted effort to achieve this.

My dad came to Britain in 1983 as I mentioned earlier. His parents sent him so he could be educated and get the best life possible. He was able to go to university, obtain a first in accounting, and follow his passion. My parents have always instilled into me the value of an education and secure a future. Many Indian parents go to extremes of not allowing children to do anything of their choice. I am lucky to not be in this position but my parents have always said to me how important education is in my life. Then it is unsurprising education is a key policy area studied by British Indians when making decisions about their children's future.

In the current day, British Indians do still place this focus on good education and excellent exam grades. 91% of British Indians achieve at least 5 passed GCSE examinations³⁰ and send the most pupils out of any ethnicity to higher education³¹. British Indians send 14% of their pupils to Russell Group Universities which is the highest percentage out of any ethnic group by 5%³². All of this data points towards British Indians achieving highly in the education sector. They are also the most likely to go to grammar schools and second-most for private schools. British Indians are willing to spend money on quality education and it something which they value hugely.

Whilst Tony Blair was a strong supporter of quality education along with his education secretaries David Blunkett, Estelle Morris, Charles Clarke, Ruth Kelly, Alan Johnson, and Ed Balls. He often used big names in this department as it somewhere with much freedom of policy. Blair and his Secretaries of State were heavily opposed to selective grammar schools and wanted to ensure equality of opportunity. Whilst this may seem appealing to ethnic minorities who could have the opportunity to stand on equal footing it was not to British Indians. Lord M Desai and Cllr Ameet Jogia both agreed that this action by Labour failed to gain support in British Indian communities. Lord Desai also notes that the removals of "scholarships for private schools were not liked." Hence this action was unpopular with the British Indians as it removed opportunity. This theme of opportunity is key among the British Indian community as it



is the reason so many of our families came to this country.

Education policy by the Conservative party has been centrally based around academies. These schools are often well maintained and aim to work in inner-city areas and remove the poor quality comprehensives. However, it did not reduce the value of grammar schools. Whilst Blair disliked Grammar Schools and private schools Cameron, May, and Johnson did not. This was the key difference as they allowed these to operate without the issues that Blair had caused. Hence British Indians still retained the option to send their child to a private school. Michael Gove worked hard to make these academies in the city of higher standards which many were. British Indians are generally urban-based where the majority of academies are and hence this change was felt directly by this group. However, it is again the rhetoric of the best education possible and the opportunities for success that were felt heavily by the British Indian community. It links into so many other key ideas. I think it is also important to stress the importance of Grammar Schools to Theresa May who strongly believed in them. She was a firm advocate for maintaining them and further expanding them and hence this was popular with the British Indian community.

In conclusion, education was very much an important area for the British Indians throughout their society. They value it as a reason they came to this country and often fall for the rhetoric on education. They like the Conservative policy simply because of the freedom it gave to private and grammar schools. These schools are capitalised upon by British Indians and Blair harmed his chances with them by hindering their existence. A Conservative Government wanting these votes must be careful around this area.

SOCIAL

When British Indians emigrated to Britain they aspired to have a better life. Aspiration is something which was central to the community when they made the journey. Ugandan Asians particularly aspired to have a better life as they were the professional classes in Uganda. They wanted to rise to the same level in Britain despite beginning at the bottom. Hence, the British Indian community see aspiration as a key value in their political identity. The language of "climbing the ladder," is important to them.

When considering which political party they naturally side with you need to look at the ideological roots. David Cameron brought in the One Nation Conservatism to the Conservative Party. Ideologically this involves being able to rise through the social and economic classes. It gave opportunities to aspire. Hence British Indians were drawn to this idea of being aspirational. In 2012 at the Conservative Party Conference in Birmingham David Cameron stressed the idea of the "aspiration nation." This idea that anyone can aspire to be anything, in an almost Disney like way, was so appealing to the British Indian community. It is also evident in the roots of One Nation Conservatism are in someone who at the time was part of a minority. Benjamin Disraeli was a Jewish man of humble backgrounds but created a wholly new ideology. His idea was that anyone can aspire to be where he is and David Cameron replicated this. Margaret Thatcher, arguably the most famous Conservative, was also heavy on the rhetoric about aspiration. She again believed anyone could make it to the top and that was the basis of neoliberalism for her. Conservatism is a complex word containing so many different schools of thought, from Neoliberals

to One Nation to Hard-Liners but what is most important is the common theme of aspiration with the group. They allowed people to aspire to be something greater and make a success of their lives. This is exactly what the British Indians wanted to do.

I think it is also crucial to link the concept of meritocracy in here. Meritocracy is the idea that the best person for the job gets it. It is a very simple concept. Whilst it has not always fitted in with the Conservative Party due to its penchant for the elite, I believe it forms the cornerstone of the party. Theresa May, Margaret Thatcher, John Major and Benjamin Disraeli are some examples of Conservative Prime Ministers from humble backgrounds. They have all been products of the meritocracy in the party; their skills not contacts won them the top job. British Indians feel the same way. They want to be able to show their skills and show they are the best for a reason. Hence, meritocracy in the Conservative Party supports this. The ideology of Conservatism is based around this key idea of "equality of opportunity." This is another key part of meritocracy.

On the flip side, Labour has not always embraced this idea. New Labour under Blair and to an extent Brown was much more Neo-Liberal in many ways and hence did not have the idea of aspiration. This aided them to retain the ethnic minority vote in the elections they faced. However, in the last 2000s, Brown lurched towards the left and alienated many of the Indian voters by further embracing socialism. Socialism ideologically believes in "equality of outcomes," which is less focussed on social climbing. It is about redistribution of wealth and high taxation which earlier was acknowledged as something British Indians dislike. Hence, they stopped voting for the Labour party economically. There were never the aspiration messages and rhetoric after Blair into the Labour party and the Brownites were unable to ignite this. It is also worth mentioning Jeremy Corbyn who focussed on "social mobility." Social mobility is not the same aspiration- social mobility is about leveling the class playing field. Richard Burgon and other prominent Labour Party politicians use this as a solution to "class warfare," not to give aspiration in the way British Indians interpret it.

Another way in which aspiration has been used is the increase in prominent Conservative and British Indian politicians. Priti Patel, Rishi Sunak, and Alok Sharma are all senior members of the government and act as role models. Cllr Ameet Jogia and the Office of Steve Baker MP both stressed the value of these role models which many British Indians aspire to be. Aspiration is not just social or economics but political in this example.

The politicians have also shown the party to be a warmer and comfortable place for British Indians to be within the party. They have shown the Conservative party to be a place where British Indians are welcomed and this does contribute to the earlier Enoch Powell imagery being removed. It is more significant than that. British Indians culturally are inclined to "trust their own." Many see Priti Patel, Alok Sharma, and Rishi Sunak as their own and feel that if they vote Conservative they are voting securely for them. It is an obscure idea but it does happen and I have seen it in my family. This idea of security does translate into electoral success at the ballot box.

The value of having Indian candidates cannot be understated. The Labour Party has been widely criticised for having no Indian candidates in safe or marginal seats. They had an under representation of British Indians in their party and many British Indians felt scorned by this. It



was like they felt they were unwelcome at the party as they didn't have any candidates. The only prominent Labour MP who comes from a British Indian background is Seema Malhotra. Despite Labour holding the upper ground by having first-ever prominent British Indian- Keith Vaz, they have now fallen behind. However, he has been disgraced and removed from the party in recent years; this inevitably affected the image presented. However, they could be seen as the original party ushering through British Indians into politics but have lost this image. Further to this on a local level in constituencies with majority British Indian communities, they are not choosing British Indian candidates. As I mentioned earlier this culture of voting for your own exists among British Indians but this has been ignored by Labour. By picking British Indian candidates in these seats they have a greater chance of winning. I will come onto this more in the recommendations section.

Whilst on a national level the party has used British Indians as a key weapon. They were visible in the election campaign and visited many of the key seats. They had Rishi Sunak compete in the debates for the Conservative Party against the other parties. They have raised the profile of the British Indians to good effect. They did have MPs of Indian origin in key swing seats however they have not analyzed the local perspective. They need to use British Indian candidates in places where there is a majority population. It feeds into this idea of idolisation in the community.

Both of these have effectively managed to win the Conservative Party more votes. The idolization is a simple and natural idea but has been the most effective of them all! It is natural and there is work to be done but I can see from my own family it has worked. My mum regularly sends me Whatsapp messages in which people are praising the work of the three British Indians in Cabinet and further to that are discussing their backgrounds. Many can relate to the journey Priti Patel's parents took or Rishi Sunak's anecdotes of his parent's racial suffering. They feel connected to them and vote for them. On the other side aspiration and meritocracy as general themes have become a key part of the messaging. They have been promoted by the Conservative Party and neglected by the Labour Party. Hence, the votes have gone away. Idolisation is a specific example of aspiration.

However, the changes to the geography and demographics of the British Indian community has also played a significant part in changing the voting behavior of British Indians. Firstly, British Indians are generally based in urban areas however, many families have now begun to move away from each other. My father and his family were all based in Hounslow growing up but now they live in a variety of areas from Amersham to Woking to Uxbridge. Ultimately they have spread out and lost some of the close family and community values which were maintained when they lived in areas densely populated by British Indians. Whilst the family might have voted Labour as a block, moving away has exposed them to new ideas. They have often chased middle-class dreams and ambitions and found these supported best by the Conservative Party. The vote is not unified but people think freely and as individuals. Also, being exposed to different areas where conservatism is the norm has also affected the voting behaviour significantly. They have seen maybe the options and reality of other changes.

There is also this generational change. British Indians are overwhelmingly a younger group of people who are now voting more freely and I acknowledged this earlier in the research. However, their identity has changed significantly. The original British Indians I would

describe as "Indians living in Britain." Many British Indians now see themselves as overwhelmingly British when it comes to identity before they are seen as Indian. This has a very interesting effect on voting behaviour. Cllr Ameet Jogia discussed the value of being "British Born." These people only know life and home in Britain and hence are more likely to identify with the British Identity. 60% of British Indians identify³³ with the "British Only" identity. Voting statistics show those who identify as overwhelmingly British are more likely to vote Conservative and hence the rise in this identity, in part caused by the geographical changes is another factor in the British Indian Community voting Conservative.

In conclusion, these two social factors have had an electoral result and effect by moving people towards the Conservative Party. They have been naturally taken to the Conservative Party through identity and geographical changes. This is nothing to do with political parties but social changes within the group which have naturally occurred. They have luckily favored the Conservatives. This sets a dangerous precedent for the Labour Party as they are losing votes as communities split up; something which is undeniably on the rise.

POLITICAL

British Indians have not just aligned socially, economically, culturally, or historically but politically too. Many of the modern British Indian political concerns are topics which align with the Conservative Party. Hence, this is another factor that influences people moving towards conservatives.

The first key political idea is that of Brexit. This was the controversy of the past three years and the British Indians are unique in this standing. Whilst those from a Caucasian background are likely to vote for Brexit but generally ethnic minorities are not. A Manchester University paper³⁴ found that British Indians are 1.6 to 2 times more likely to vote for Brexit than any other ethnic minorities. Hence the Conservative Party, being the strongest party on Brexit, are going to gain the votes of the Brexit supporting British Indians. The Conservative Party went into the election with the slogan "Get Brexit Done," and for those British Indians who voted for Brexit supported this heavily. It was at 30% for British Hindus and 35% for British Asians. Hence there are 30% of the British Indian population immediately attracted to the Conservative Party. Whilst the Brexit Party may seem like an even more natural avenue they were not prominent enough to take voters away.

Brexit generally appealed to the British Indians for a pair of reasons. Firstly, British Indians do not like to waste money. The Leave campaign argued that the EU was a waste of money and British Indians understood and responded to these claims. Further to this the immigration issue was also very important. I will explain this in more depth below. Both of these ideas are important in the Brexit argument but also the wider political argument.

Another key and relevant political theme is immigration. There is an immediate irony in immigrants wanting tighter control but as you delve into the Australian Immigration System you see that it does not limit immigration but create a level playing field. This has been exemplified by the Brexit revolution. David Cameron came to power promising immigration controls and quotas. Whilst this was possibly not something British Indians consciously liked they did find it appealing. Boris Johnson presented the Australian Style immigration system as a solution; this is now Conservative Party policy and appeals to the British Indian community. This was also stressed by Cllr Ameet Jogia who said this



was a "prominent" issue on the doorsteps. He found this to be a key concern of many British Indians and something they wanted to implement.

Another recent point was Priti Patel's speech in Parliament on racism. She was candid in her response to Labour MPs over racism describing her time being called a "paki." A disgusting and abhorrent word but something which myself, my family and almost every British India has been called. Her rhetoric and the Conservative party rhetoric has been more sympathetic to the British Indian community; naturally this appeals to the group.

Both of these ideas fit naturally into the Conservative Party, not the Labour Party. They are more pro-Europe and pro-immigration and this is something the British Indians generally do not favour.

Whilst these key political issue do not always dominate the landscape they have in recent years. Immigration since 2010 and Brexit since 2015 are crucial items which the Conservative Party policy aligns with the opinions of British Indians. These issues have affected the vote share in constituencies such as Harrow East. These ideas are not always at the forefront of the minds of British Indians, but they do force the voting behaviour to move towards the Conservative Party.

CULTURAL

Many of the cultural values that are important to British Indians are also values that are embodied in the Conservative Party. Values which are the part of Hindu culture and Indian culture play a significant part in the social and political values of the Conservative Party. Values like this should not be understated as linking to the Conservative Party to the British Indian and Hindu community.

The first value is that of family. When I interviewed Jonathon Lord MP he stressed that "family values are central to the community." The idea of stable family culture is something that is key to British Indians. Indian culture is generally very backward with the idea of homosexuality, blended families, and co-habitation being strongly complained against. It is seen as immoral and wrong in many ways by the elders in our society. They believe in simple nuclear families. This is similar to the values of the Conservative party. Ideologically the party does value tradition as the ideal. Tradition is a flexible term but many British Indians have customary family and religious traditions which they follow intensely. Hence the marriage of conservatism and British Indian culture is natural.

The other key area of culture in which there is agreement is that of law and order. The Conservative party is also famed for having a strong belief in a tough justice system but also retaining high levels of law and order. In 2019 they introduced many policies including longer punishments for a variety of crimes and more prisons which aimed to achieve a tougher justice system. The Conservative Party belief in firm punishment and justice. This is echoed by the beliefs of the many Indians and Hindus around the country. The belief in karma informs much of the British Indian view. Karma is a cosmic principle of equality and justice. It states that whatever one does upon another will be received upon them; put colloquially: what goes around comes around. This links into justice and equality in punishment. Hence, many believe that prisoners get easy punishments and feel they should be harsher. Whilst it may sound cliché Indian parents are often strict with children.

This belief in firm punishment is reflected on a wider political scale.

They are more naturally drawn to the Conservative Party than the Labour party who are more focussed on restorative justice. Hence this is another way in which cultural values marry up. In conclusion, culturally the Conservative Party and British Indian are natural together and it is down to the party to show and prove this.

RECCOMENDATIONS FOR THE FUTURE

WHERE NEXT LABOUR

British Indians are a complex ethnic group with a myriad of different interests. The overwhelming theme is a movement towards the Conservative Party and the data and political evidence show this. Whether it is in the social, cultural, political, economic, or historic factors British Indians are being pulled towards the Conservative Party. It is undeniable Labour has some areas which appeal to British Indians but these have diminished, especially as the party has embraced radical socialism under Jeremy Corbyn. However, the Labour Party and Sir Keir Starmer have acknowledged these issues very early in his leadership. He has tried valiantly to understand and work with the British Indian voters as far as possible. The Labour Friends of India are the central British Indian organisation within the Labour Party who are driving for the representation of the Labour party. They are trying to further their interests in the Labour Party. Keir Starmer has also worked to expel racism in all of it's forms from the party; it is another way to retain ethnic minority support on a broader scale.

Inevitably the move over Kashmir, which was outlined in-depth earlier, was a frustrating moment for British Indians across the country. However, this was felt heavily by the Labour Friends of India; they had been marginalised by a divisive issue. However, Keir Starmer has held a zoom meeting and changed Labour's stance on Kashmir in the past few weeks. He said that it was a "bilateral issue," on April 30th after meeting with Labour Friends of India and Angela Rayner. Corbyn alienated British Indian voters with his harsh words over Kashmir as I explained earlier. However, Starmer has tried to recognize that this minority is the most populous and important in his bid to regain power. It is a minority that has cost Labour power in the last decade. He has quoted the issue as "constitutional," which is exactly what is maintained by the Indian community. With this being his first move in this area it highlights the significance he places upon the issue. Evidently, he sees it as something which is a "turning point." However, there has already been a major issue. Pakistani groups within the Labour Party are arguably more important and there are more Pakistani origin MPs. MPs like Tariq Ali have been critical of Keir Starmer in the press and have tried to force a "U-Turn" over this position. They feel that it is a moral issue. Starmer, despite his comments on April 30th regarding this issue, has made a largely unnoticed U-Turn. He has proclaimed to the Muslim Council of Britain that "Our Position on Kashmir has not changed." He further commented that "India and Pakistan need to work together with the people of Kashmir." This is a subtle call for self-determination. Whilst being less brazen he has not officially changed the position. This position cannot be maintained of appeasing both Indian and Pakistani calls within his party. A number of Labour MPs of Pakistani origin have been angry about this move despite no official change. I suspect his



backbenchers force him to retain this position; it is unlikely he will be able to withdraw himself from this issue. Kim Johnson, MP for Liverpool, spoke to me and said that her constituents are "highly concerned." It is surely impossible for Keir Starmer to maintain this intermediate position on a contentious issue. Labour needs to find a way to kill the issue and stop the media storm it has created. By moving away from the issue and using a softer language he will be able to try and please everyone. Ultimately they have to be on one side of the barrier and that will be one of self-determination. However, the right way to resolve this could be caveating it. Suggesting the wishes of the Indian Government and history will be equally respected rather than focussing on the rights of Kashmiri people entirely. By balancing their approach and giving candidates a form of defence by suggesting it is a trifold idea they will be able to appease the British Indians. By respecting both the issues on either side, combining them and possibly using the United Nations as an intermediary could prove an effective tactic. Hence, this is my first suggestion for Labour is to come up with a balanced Kashmir stance which rightfully respects both sides of the debate- history, politics, and human rights. He can still condemn what he considers as atrocities but maintaining a balanced approach is vital. The most important takeaway is to acknowledge both sides of the argument then try to balance them accordingly.

However, there are obviously other areas in which British Indians and the Labour party have moved away. I think the primary issue is to build a relationship with Narendra Modi. Starmer has already begun this process by calling India a major "post-Brexit trading partner." He has recognised David Cameron won a significant proportion of the vote from British Indians after hosting Modi in 2015 and he would like to use the same thing. Indians are proud of their homeland and having a good relationship makes them very proud of a party. Modi's endorsement was also vital for Cameron and Starmer hopes that he can compete with Boris Johnson for the crucial endorsement. He does have a complex job with the Labour Party having many critics of this policy. I am not naive to the fact it will be difficult but the suggestions will make his relationship with British Indians stronger.

Starmer does also have the "professional image," needed to win the British Indian vote. Professionalism is something which British Indians look for in politicians- they want them to be educated, intellectual, and professional politicians. Whilst Johnson may not always appear like this he does have an Oxford background, and is by no means incompetent intellectually. Starmer also has the same and his background will support his image. Competence is something that is evident in Keir Starmer. He must maintain this image to help to gain votes. Corbyn did not manage to give this professional image which is vital to winning the British Indian vote. Many of them are professionals and will vote for the same. However, Starmer can also use his background in law to appeal to the British Indian desire for law order. He can appeal to this social element of their being to try and draw them in through this work. He was Director of Public Prosecutions and using this experience to suggest he will be able to handle crime would be an effective strategy.

The direct political policy should not be driven by the desire to please a single ethnic group as he would be pulled in all sorts of directions. He would not be able to appease every single group because ultimately they all want entirely different things. However, rhetoric can be specifically used in an ethnic group. On a local level, Jonathon Lord MP described how when he spoke at the Surrey Hindu Cultural Association

he changed his rhetoric to suit what he saw as the requirements of the Hindu Population. On the other hand has also described the Labour Party candidate failing to do so especially regarding Kashmir. When you are at an Indian event focus on your policies that appeal to them like you would at any event. This messaging effectively placed was something that feels self-explanatory but Jeremy Corbyn and Ed Miliband failed to do. For example, focus on the economic strategy for the business which will appeal to British Indians when speaking to them, or law and order background or education investment. Speak about these vital things when working with the community. Education is another policy area in which he could be very effective. He attended Reigate Grammar School which was a Grammar School for a period he was there. Indians are acknowledged earlier support Grammar school. He needs to stress this point as it is an area of mutual bonding; he can begin to create a relationship with the group. By creating common ground with this ethnic group he will be able to engage them much more effectively than he would be able to do so otherwise. Again he needs to give the impression of "one of their own."

On the same idea, his candidate selection needs to be shrewdly played. Where there is a large British Indian or any ethnic minority community, select a candidate who can connect with the community. Statistics show ethnic minorities are subconsciously more likely to vote for that candidate. This is something that is not overly complicated by shrewd electioneering. It plays into the idea of "one of their own." It is not overly complex and a simple and easy recommendation.

Finally, I would urge Keir Starmer to try and personally engage with the community. David Cameron attended Diwali events, held party receptions, and spoke to the community. He was lucky to have the expertise of Lord Dolar Popat however Starmer can use his own parties knowledge and the general ideas from Lord Dolar Popat. By hosting Diwali events he begins to gain the loyalty of voters slowly and surely. Whilst this is not always going to be easy it is doable. By engaging the community he can show why the Labour party is a viable option. He needs to present himself as a friend of the community and someone who understands the critical issues. He can show British Indians that they are a vital part of the society he envisages for the future. He needs to work in places where Labour has been suffering from reduced majorities such as Leicester, Harrow and Watford where they have lost seats. By electioneering early with the community he can target them and I believe if they do it correctly they are vulnerable. Rhetoric is important here too. He needs to remind them who fights for ethnic minorities and who puts their interests first. He can use the recent developments in the Black Lives Matter movement as a catalyst. Events like this are the basis for community and local relationships.

Finally, those MPs with large populations of British Indians need to understand the communities they work in. This recommendation was supported by Tony McNulty. He suggested there needs to be a "strategy and vision that can appeal to communities." These are exactly the changes which need to be implemented. On a national level MPs need to be given clear instructions on how to engage with our communities. The leadership need to take responsibility for this issue however, it is also down to local councils. If they can along with the associations work with the MPs on community engagement then there will be a greater level of success for the Labour Party on a national level. Focus on this element is not one-sided.

In conclusion, Labour has a difficult job winning these seats back



because they have failed in the last 10 years. However, Starmer does have the credentials to manage this by clarifying balanced positions and engagement. A variety of smaller measures will win back these voters if they play it correctly.

WHERE NEXT FOR THE CONSERVATIVES

The Conservative Party has been a success story overall with British Indians in the past decade. They have many more votes however, there are still seats in areas such as Leicester, Derby, and Brent where they have work to do. In all these regions, they have decreased majorities of senior Labour party figures like Jon Ashworth, Dawn Butler, Diane Abbott, and Barry Gardiner. These seats are now being contested to a greater extent and with even more targeted work towards British Indians will be a huge threat.

The Conservative Party needs to continue to engage with the community in the same way they have over the past decade. I would consider setting up an event to praise and accept the contribution British Indians make to the country. British Indians are leaders in the professional services and inviting leaders to reception to honour the history of immigration would be a vital step. This could continue to build links with senior leaders but also individual leaders in communities. We need to invite Punjabi, Gujarati, Kashmiri, and Goan immigrants to celebrate the work of British Indians. Recognising the diverse culture within the British Indian sphere will be an effective strategy. A huge part of how to engage British Indians is the validation. This event could be led by the CFI to provide a celebration of what British Indians are to the country. It is the cultural value of this when the community feels like they are valued by the party and they will repay this loyalty at the ballot box. By also honouring British Indian culture by continuing Diwali and temple visits it shows a sustained interest, not just at election times but all times. British Indians know their votes can change elections and hence they are valued highly. They do not want superficial engagement but genuine engagement. I would also consider the value of street art as a cultural unification. By commissioning a mural or statue celebrating British Indians this will be well received by the population. It is the little actions that mean the most to the community that has suffered greatly. Colonisation is another issue which I would argue an acknowledgement and apology for could be beneficial. Many Indians feel angry about this so by apologizing for the obvious mistakes could be welcoming and humble. I have seen murals which are dedicated to cultures and there should be one commissioned around the country. By depicting the value of British Indians in our multicultural society it will be a feel-good and easement factor not just for British Indians but all ethnic minorities. It is a genuine way of changing the field of play for the better. I believe it will make people feel that the Conservative Party is engaged. Like the song "Neelam Hai Asama," they need similar initiatives to keep the community going and engaged. This will be a serious piece of progress for the British Indian community by keeping the engagement up. Finally, Indian Independence Day is often understated by the political parties- an event celebrating this could be a strong movement in India and Britain. It would also acknowledge the difficulties of empire. Empire has strong connotations for many British Indians; acknowledgement of mistakes may alleviate some of the pain and anger.

I also believe that shrewdness in candidate selection must be applied.

British Indians will respond better to the Indian candidate than they would to a British candidate generally. They feel unity and common ground- they will be representing us the best as they are one of us. It is not the most logical thing, but it is a psychological idea which we should embrace as soon as possible. It is a requirement for this to happen in my opinion because it is the best way to win seats. In places like Leicester compete there with British Indian candidates as much as possible because it will aid out the cause. It is not a complex electoral strategy and it is very easy to implement in constituencies.

I would also argue that they need to use the right rhetoric which appeals to British Indians. As I outlined earlier aspiration and education are vital for British Indians. So, talk about aspiration when addressing British Indians like Jonathon Lord MP did. It is a key technique to show the British Indians why they should vote for you. The importance of why cannot be stressed enough- if you have rational voters, they will be weighing up pros and cons. It is the party's job to add the pros column. It is about focussed campaigning on the type of person they are and aim for that. It will support the aim to gain more of the vote which they haven't always won. They need to begin to work with Indians across the country and use the visible figures they have as role models. By sending Alok Sharma, Priti Patel and Rishi Sunak into constituencies where they can campaign and connect with British Indians who have similar stories will undoubtedly be a prudent tactic.

The Conservative Friends of India have a large role to play and have resources to aid this. They could focus on exploring which seats they want to fight in and aid British Indian seats. By making themselves a presence at local meetings and working with colleges and communities they can show what is out there. They should also consider how they can promote British Indianism in the right seats. By possible working with the party to suggest their own bank of candidates for British Indian majority seats and they can be involved with the process. However, I think the central idea is to integrate into communities. By working with groups like the Surrey Hindu Association or other local groups they can hold and sponsor events. By bringing big figures with them the community will feel like they are being directly addressed by the most senior politicians in the country. They can promote interests.

They should also from an electoral point of view try to encourage the party to work with the British Indian community during election time. By possibly trying to get British Indian figure from the party into the communities which they have the greatest knowledge about is an idea. It would be great to see them do this to use the expertise of members in communities to work out who and where they can have the greatest impact. They should also work with candidates in Indian areas to suggest what to focus on when campaigning and talking to British Indians.

My most significant suggestion for this group is that they should try to offer services to British Indians on a wider cultural scale. Using the expertise, they could sponsor local community events and show the engagement in local communities. Whether this involves Diwali or Navratri functions they could provide a location, a venue, a guest speaker, or mehndi (henna) services. Asking members to volunteer expertise and support might be a unique and exciting way of campaigning in the key swing constituencies. It is not a traditional political movement, but culture is one of the most important parts of British Indians. Hence, they involve politics and culture. They could also generally be an avenue of political support by referring the community



to the correct people- from the example the MP or foreign office over visa concerns. They will not forget the support you have offered, and it will make a huge difference for them.

In the past, the Conservatives have had an issue with racism. They still face serious challenges from Islamophobia within the party. In the current situation the Black Lives Matter movement has shown rapidly increasing momentum. They must reconcile with all races over the scandalous stop and search policy but more significantly, the tarnished history. Responding to this issue is a must; they need to be proactive. By holding consultations or engagement sessions to understand concerns they can address them. They must, at least to save face, make a change.

Finally, the emphasis moves towards the local MPs and candidates. When campaigning they need to work with the British Indian population by talking to them but also treating them on equal footing and in the same way as everyone- just because they are a minority, they don't want special treatment at election time. Chris Grayling MP commented in response to my questions that he believes they want "equal footing," and I agree with this. He did agree that the events are crucial to raising support. On the doorsteps show why you can specifically aid their community and concerns. Talk to them about what matters to their community whether it is having their own space or racism on the street. They do need to deal with issues that matter to them like any other constituent, but they have different concerns. Realise this and manage them effectively. It is simple to do and a great strategy. Further to this, speak about issues which you know matter to them like aspiration, family and education, Why the party is the best on these issues is the emphasis you need to place. MPs when campaigning can do all these things but actions when in office are crucial, if they can make a focussed and real effort to engage with communities like Tony McNulty mentioned earlier, they will be far more successful.

In conclusion, British Indians and the conservative party have begun to grow closer. The work so far is great but there are simple additions to secure this vote. Strategic candidacy and the work of the CFI can win the party many constituencies which were unattainable. The changes are easy and create efficient electoral practice. It is important to note the Conservative Party do not have all the British Indian vote and still need to address certain concerns.

CONCLUSION

British Indians are complex. When concluding it is vital to caveat my work. I am a 17-year-old student exploring a deeply complex topic which has many different strands. I have had amazing support and I credit those who have been especially important below. My research has been hindered by the coronavirus crisis and I haven't been able to explore as many different areas as I would like. However, this does not take away from the fact that I am a politically active British Indian that has experienced much of our culture. I have a wide and diverse family which I am lucky to be able to draw upon. They have helped me a lot with their advice and experiences of the political culture and I am lucky to have had this as a support for my project. British Indians, themselves cannot be constrained as single block vote or ethnic group. Every single person I have interviewed has agreed with this first premise. British Indians all have entirely different backgrounds and social desires. These differing backgrounds and locations mean there is not a single strategy

which you can conclusively say will win the British Indian vote. It is not going to work so you need to be flexible and diverse. These different opinions and ideas will need to be catered for in a variety of ways. Political candidates and parties can use a variety of methods that will aid you in trying to win the vote. There are a variety of key factors which I am going to summarise by generation.

The older, first-generation immigrants are focussed on history. This group values who let them into the country and have the best memories of their homelands. They often feel like visitors to the country and till reminisce about home. Hence British Indians in this group overwhelmingly vote Labour because they have driven the immigration change and made them feel more welcome, to begin with. History is the driving factor in voting behaviour which is unchangeable. They feel the effects of Enoch Powell and do struggle to manage this. Hence, this group is solidly set in their ways and unlikely to change. Hence, this group of the British Indians solidly vote Labour however being the older generation they are sadly passing away and part of the reason the vote for Labour is diminishing. However, whilst the physical voters are changing the psychology of British Indians has not changed; the Conservatives cannot lessen the efforts.

However, all the other generations are wholly different in what drives their voting behaviour. Social, cultural, economic, and political factors all contribute in different proportions. It makes it near impossible to manage all these expectations. Generally, the prevailing theme is cautious economic policy with a focus on secure and stable systems. This is similar to the economic theory of austerity. Many British Indians holds close the value of saving not spending- this is what they were forced to do growing up. Hence on a wider scale, this is applied. The keyword around the whole of this is engagement. Making the community feel part of British culture and combing identity. It is about the unification and whilst values are similar, they need to feel welcome. Generally, this has been achieved across the board and then you drive deeper into policy. Policies that British Indians like are the ones which are generally Conservative, but they were, blurred with New Labour. Since the socialist movement of the Labour party and widening of the political gap, this has exposed to British Indians why they are closer to the Conservative Party. Inevitably this will change with shifting political parties and Keir Starmer is likely to try and move Labour back to the centre. This will test the British Indian bonds with the Conservative party.

Tactics to engagement vary across the political parties. Labour must win these voters back politically and over Kashmir. It is a difficult task to manage the party's variety of ideas and backgrounds on contentious issues. The Conservatives must keep going and use the CFI who has the knowledge of the local communities which need careful management and care. They need to capitalise on the resources they have within the party.

Harrow East is a fine and shining example of what has happened over the past few years. This is where British Indians have moved away to Conservative messaging and is a tribute to the work of Bob Blackman in the local community.

It is also important to accept the diversity of flexibility of British Indians. Whilst other ethnic groups can be categorised as a single group you cannot easily do this with British Indians. Generally, politics in been much more flexible and fluid. It is crucial avoid the stereotypes of everyone is this minority votes this way. This was acknowledged by



Tony McNulty in his notes to me where he describes the “fluidity” of the electorate. Further to this he urges a resistance to stereotyping. So, whilst the project as whole categorises British Indians and types how they vote. There will always be exceptions in every minority, and these just must be taken as they are. Especially in a diverse and settled group like British Indians there are a growing number of anomalies from the trend.

Overall, my overriding theme of the project is that British Indians have changed the wider political spectrum and are complex beasts. They have moved towards the Conservative party now, but this is an ever-changing scenario. They have shifted the political standing in the United Kingdom much further towards the Conservative party. 1.4 million might not seem like a big number in the context of the United Kingdom but these historically, culturally, socially, economically, and politically diverse individuals have an overwhelming impact on the political system. Gaining their votes will determine a significant part of British politics as they are a large percentage of swinging voters. It is important that this minority gets the representation they deserve and continue to flourish in Britain.

WITH THANKS TO:

Lord Meghnad Desai

Lord Dolar Popat

Cllr. Ameet Jogia

Cllr. Reena Ranger

Jonathon Lord MP

Chris Grayling MP

Kim Johnson MP

Bob Blackman MP

Dr. Martin Offord MP

Shailesh Vara MP

Cllr Vina Mithani

Tony McNulty

John Austin



The New Cold War: Rising tensions in the Arctic Circle

Cameron Philp



Royal Marines during arctic warfare training in Norway - January 2020 – Crown Copyright

The Arctic has undergone a rapid transformation from a barren wasteland to a region of enormous economic and strategic opportunity in the last two decades. This report begins by identifying and analysing the causes and effects of climate change in the Arctic then the consequent rising tensions between states. I use this information and additional research and knowledge to determine whether these rising tensions will result in conflict in the Arctic Circle.

INTRODUCTION

Unlike the Antarctic and many other parts of the world, the Arctic is a region of unclear territories, rapid change and emerging economic and strategic importance. The Arctic Circle is the northernmost line of latitude on the globe and consists of a deep ocean covered by a drifting expanse of frozen seawater. This ice cap is the major feature of the area and it expands in winter as the sea freezes and reduces in size in the summer as the ice melts. Iceland, Denmark (through Greenland), Norway, Sweden, Finland, Russia, Canada and the United States

are the eight 'Arctic States' that are located within the Arctic Circle. Approximately 4 million people live and work in the Arctic¹.

The extent of the Arctic ice cap has been decreasing significantly in the past few decades due to increasing average global temperatures. This rise in average temperature of the Earth's climate is known as global warming and the Arctic is warming at a rate of almost twice the global average². Global warming is caused by many factors including the release of heat-trapping gases, such as carbon dioxide from the burning of fossil fuels in power stations, that leads to a greater 'greenhouse effect'³. The 'greenhouse effect' is the warming that happens when certain gases in the atmosphere let light in and out but trap heat. Since the Industrial Revolution, the actions of humankind have had an increasingly damaging impact on the planet's natural environment through an enhanced greenhouse effect. This has led the Arctic ice sheet to melt significantly and continues to at a terrifying rate due to increasing average temperatures. The last three winters in the Arctic have been 6°C warmer than the average for the region⁴ and between 1982 and 2012, Arctic sea ice coverage decreased by over 40% from 8.3 to 4.7 million square kilometres⁵. At the current receding rate, an ice-free Arctic is very likely in the next century and ice-free summers within the next few decades. This has many negative consequences. However, the decreasing ice coverage has meant resources previously inaccessible or too expensive to access are becoming available and commercially viable for exploitation.



Map of the Arctic Region © Swoop Travel Ltd

NEW RESOURCES AND OLD TERRITORY

One of the features of the 1982 United Nations Convention on Law of the Sea was the introduction of jurisdiction of an area 200 nautical miles beyond the coastline of all coastal nations called the 'exclusive economic zone' (EEZ). In the EEZ, the coastal state has sovereign rights for the purpose of exploring, exploiting, conserving and managing natural resources, the ability to conduct marine scientific research and to operate ships, aircraft and submarines⁶.

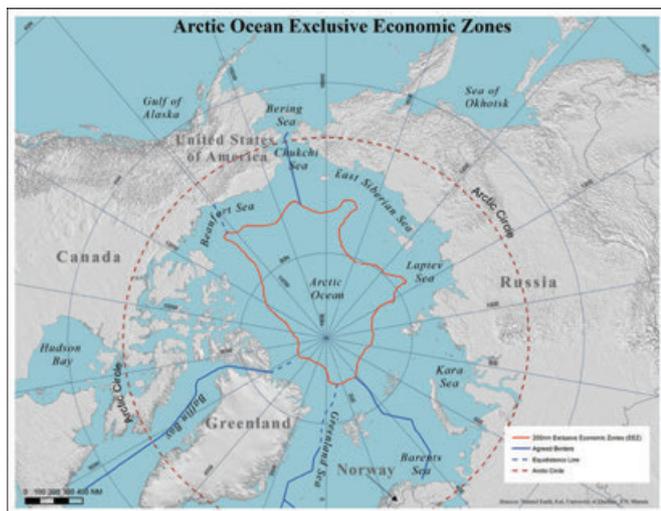


Figure 1

The North Pole and surrounding waters are not currently owned by or part of the EEZ of any country (figure 1) – it is 'international waters' or 'the high seas'. All nations are able to navigate, fly over, lay cables, fish, conduct scientific research and obtain natural resources in international waters according to UN Maritime Laws.⁷

The main advantage to the EEZ is the exclusive access to resources it grants. In some parts of the world, such as the South China Sea, the primary resource is fish whereas in the Arctic it is oil and natural gas. The Arctic Circle is estimated to have approximately 13% of Earth's undiscovered oil reserves - the equivalent of 90 billion barrels of oil – which is worth over US\$5.5 billion at January 2020 prices⁸. In comparison, Canada holds 168.9 billion barrels and the US 50.0 billion⁹. This oil has been inaccessible in the past because the Arctic is an incredibly cold, isolated, dark, dangerous and expensive place to obtain it. The harsh environment means only equipment designed to withstand the temperatures can be used, the volatile ice sheet can damage offshore facilities and slow the transport of personnel, equipment and oil and long supply chains to the refineries requires a larger amount of equipment and a greater inventory of vehicles. Workers demand higher wages for working in the tough Arctic environment as well¹⁰ and infrastructure is almost non-existent.¹¹ These Arctic-specific costs of production make oil exploration and production in the Arctic 50-100%¹² more expensive than other areas of oil production such as the Middle East.

As the ice sheet has decreased, oil can be now obtained at lower costs of production than previously. This is why only recently has drilling for oil in the Arctic become a profitable venture for oil companies around the world. The same is true for natural gas, as the methods of production are similar. The Arctic has an estimated 1,669 trillion cubic feet of

gas, worth approximately US\$4.2 trillion at 2019 prices and equal to 24.3% of the world's current known reserves. That's equal to 500% of U.S. reserves, 99% of Russia's reserves, or 2,736% of Canada's natural gas reserves¹³. There are also masses of other natural resources including gold, diamonds, copper, iron, zinc and uranium which are also able to be viably mined at these lower costs of production.

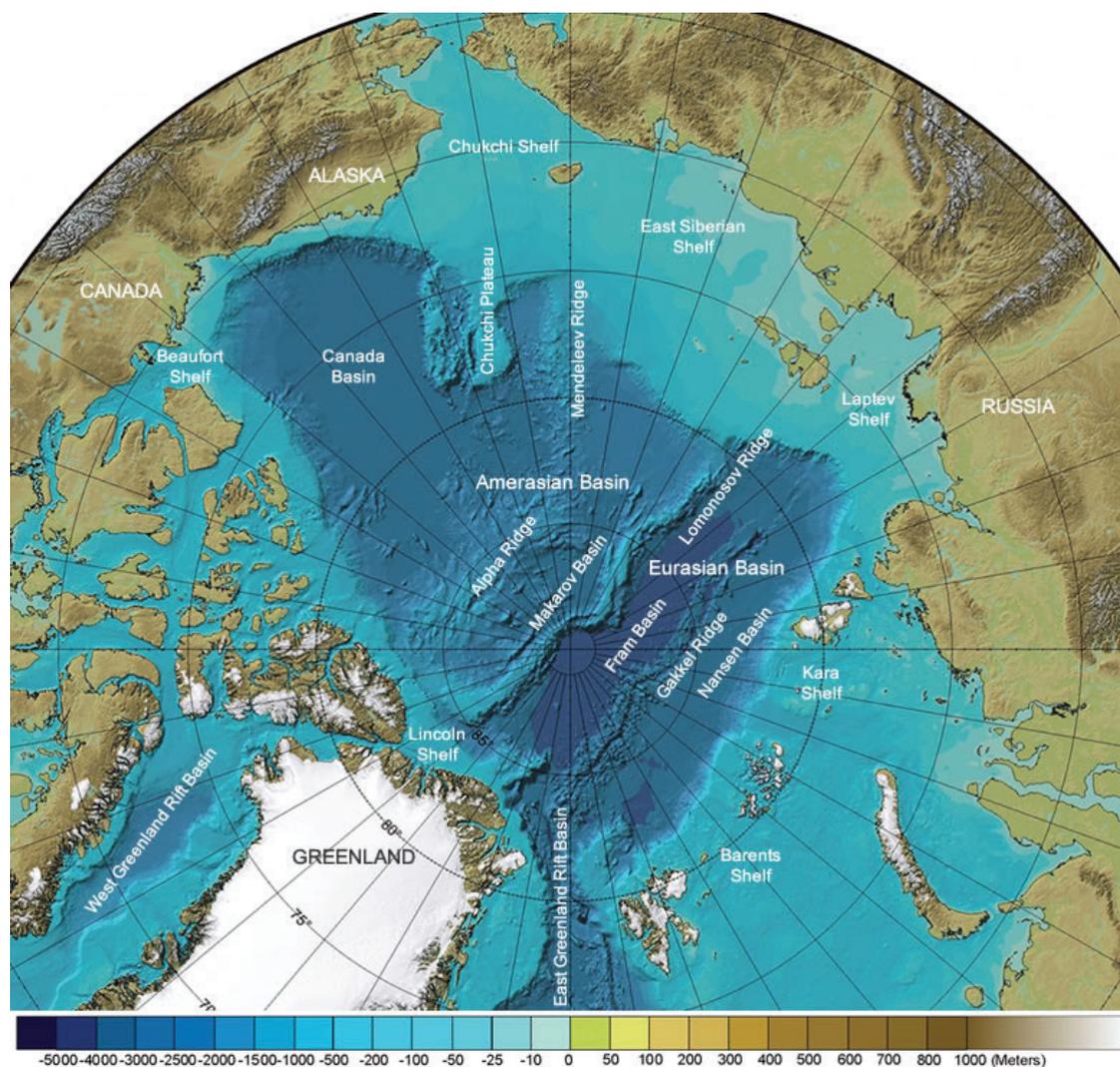


Figure 2: Shipping routes in the Arctic Circle
Source: Central Intelligence Agency (CIA)

New shipping routes are becoming available too, heralding a new era of shipping on the top of the world. In September 2017, a Danish container ship became the first to complete the Northern Sea Route (figure 2), travelling from East Asia to Northern Europe over the top of Russia. The route was 10 days shorter than the standard route through the South China Sea, under India, through the Suez Canal and the Mediterranean and finally around Spain and France. In 2014 a Canadian vessel became the first to traverse the Northwest Passage (figure 2) over Canada and Alaska on a journey from Quebec to China.¹⁴ The journey took 2 weeks less than the 41-day standard trip through the Panama Canal. Arctic shipping routes became cost-effective only in the summers from 2010 as icebreakers were still required in the winters and more and more vessels are making the journey unescorted each year.¹⁵ As 90% of the world's trade is transported by sea,¹⁶ shipping routes are essential to the global economy and consequently the routes across the Arctic have huge strategic and economic value. These routes will cut hundreds of thousands of dollars off fuel costs as well as avoid East African piracy and maritime choke points¹⁷. The economy of the Arctic could be transformed in a similar manner to how the Middle East was by the Suez Canal. The huge economic and strategic imperative from the creation of the Northern Sea Route and the Northwest Passage as well as the lower costs of extracting natural resources from beneath the Arctic Ocean have led to a race for Arctic domination between the Arctic States and other nations in a region that until recently was desolate¹⁸.

RIVAL CONTINENTAL SHELF CLAIMS

Another feature of the Exclusive Economic Zone (EEZ) in the United Nations Convention on the Law of the Sea (UNCLOS) was the ability for a nation to expand its exclusive economic zone. If the continental shelf of a nation extends beyond their EEZ, the nation can make a claim



International Bathymetric Chart of the Arctic Ocean annotated with the names of seafloor features

to it. A claim is submitted accompanied by evidence to the Commission on the Limits of the Continental Shelf (CLCS) for a lengthy review. If successful, the state may obtain exclusive rights to the resources on and below the sea floor in that area.

In order to maximize their share of the Arctic's enormous resource wealth, the Arctic States have made multiple continental shelf claims. Many of these claims overlap each other and are the main cause of the rising tensions in the Arctic Circle. Canada, Denmark, Norway, Russia and the United States all have continental shelf claims that have been submitted since 2006 including as recently as 2019. Notably only Canada submitted claims before 2006, emphasizing the huge change global warming has had on international relations in the Arctic and the prevalence of the topic.

Russia has been the most active in staking its claims. Russia has conducted extensive research of the sea floor of the Arctic Ocean, their main aim to prove the Lomonosov Ridge, an underwater 'mountain range' stretching over the Arctic Ocean, is an extension of the Eurasian continental shelf and therefore obtain exclusive rights to the sea floor extending all the way to the North Pole (figure 4). This would give Russia exclusive rights to almost half the Arctic Ocean in total, and therefore billions of tons of resources and a large proportion of the mineral wealth. Its 2001 claim to the ridge was unsuccessful due to lack of evidence though in 2015 Russia submitted another bid to the UN with more evidence.¹⁹ This submission included the Lomonosov

Ridge, Mendeleev-Alpha Ridge and Chukchi Plateau as well as parts of the Amerasian Basin and Chukchi Shelf (figure 3). In addition, Russian explorers planted a titanium flag on the seabed 4km below the North Pole in 2007 in what was dubbed a "15th century" move to further this claim²⁰.

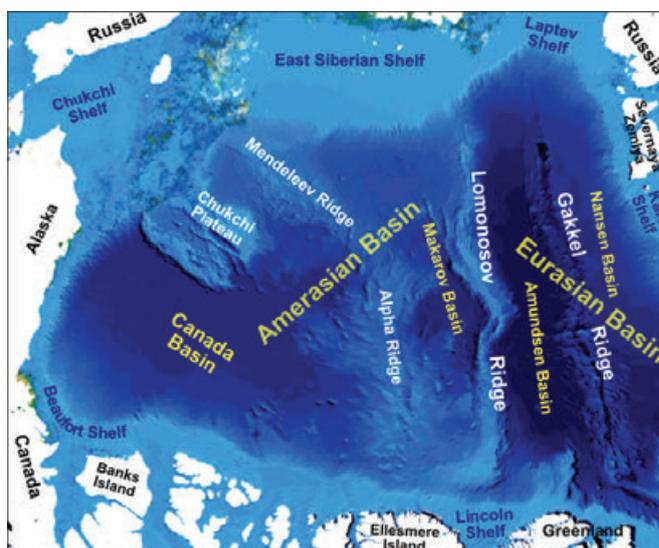


Figure 3: Main bathymetric features of the Arctic Ocean Source: Wikipedia Commons - Mikenorton

Denmark submitted a claim for the Lomonosov Ridge (figure 4) to the Commission on the Limits of the Continental Shelf on 15 December 2014 which conflicted with Russia's claim. It argued the ridge is "both morphologically and geologically an integral part of the Northern Continental Margin of Greenland"²¹ meaning that it is an extension of the Greenland land mass. The nation presented evidence it had collected since 2002 to support its claim to approximately 895,000 sq. km of sea floor²² - 20 times the size of Denmark - that extends over the North Pole more than a thousand miles from the nearest point on the Greenland coastline to the edge of Russia's current exclusive economic zone (figure 4).²³

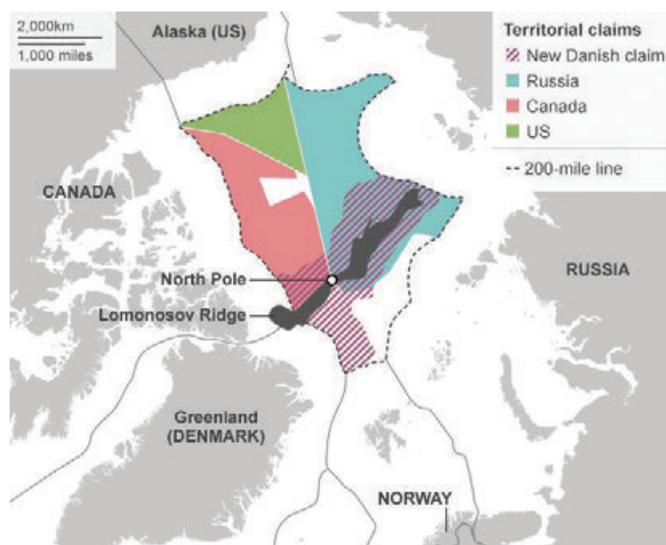


Figure 4: Source: BBC

Canada have claimed the 'Central Arctic Plateau' (which includes the Lomonosov, Alpha and Mendeleev Ridges) and the Canadian and Amerasian Basins are a continuation of the Canadian landmass and a part of its continental shelf²⁴ (figures 3 and 4). Research was conducted for only two eight-week periods a year between 2008 and 2018 due to the harsh conditions and the research in the Eastern Arctic region was unreliable due to thick ice. While this limited the amount of evidence available for them to use, Canada submitted the 1.2 million sq. km²⁵ claim on 23 May 2019, just over a year from writing. The claim also conflicts with and Denmark's and Russia's claim, which is of a similar

size. Importantly, the Amerasian Basin contains 9.72 billion barrels of crude oil, the third greatest of the known petroleum regions in the Arctic, worth over US\$600 billion at January 2020 prices.

The United States of America worked with Canada between 2008 and 2011 to research its continental shelf. From data collected by the US Geological Survey (USGS) on this expedition, it was discovered Arctic Alaska has the largest amount of crude oil of the petroleum regions in the Arctic (29.96 billion barrels of crude oil, three times as much as the Amerasian Basin which Canada has laid claim to) and a significant volume of natural gas (221.40 trillion cubic feet)²⁶. Their claim focuses on the area between Canada's and Russia's claim in the Chuckchi Basin (figures 3 and 4). However, while the US recognizes the United Nations Convention on the Law of the Sea, they are one of the very few nations that has not ratified it and as such is not able to make an extended continental shelf claim to the UN. Therefore, for the US it is incredibly important that the Arctic remains as open as possible not only so it is able to obtain as much of this oil and natural gas as it can but also so it is able to protect its Arctic assets and national security without resistance.

Norway is another Arctic State to make a claim to the CLCS. Their November 2006 submission claimed areas of the Barents Shelf, North East Atlantic Ocean and the Eurasian Basin are part of the continuous continental margin of Norway (figures 3 and 4)²⁷, conflicting with Denmark's and Russia's claims. The largest area they claimed was a part of the Eurasian Continental Margin consisting of the area adjacent to Norway and the Svalbard Archipelago from the North Sea into the Eurasian Basin before the Lomonosov Ridge. (figures 1, 3 and 4). The Norwegian Margin and Barents Platform regions included in the claim are predicted to hold approximately 4 billion barrels of crude oil as well as 60 trillion cubic feet of Natural Gas according to the USGS (figure 5).

However, as with all contradicting claims, the nations must negotiate their new territories because the CLCS cannot approve the claims until the borders have been agreed upon between themselves. In addition, Canada, Denmark, Norway, Russia and the United States agreed at the Arctic Ocean Conference in May 2008 that all demarcation issues should be resolved between the nations with conflicting claims²⁸ and not through the UN. But the nations are finding it difficult to agree, and this is the primary reason for the rising tensions.

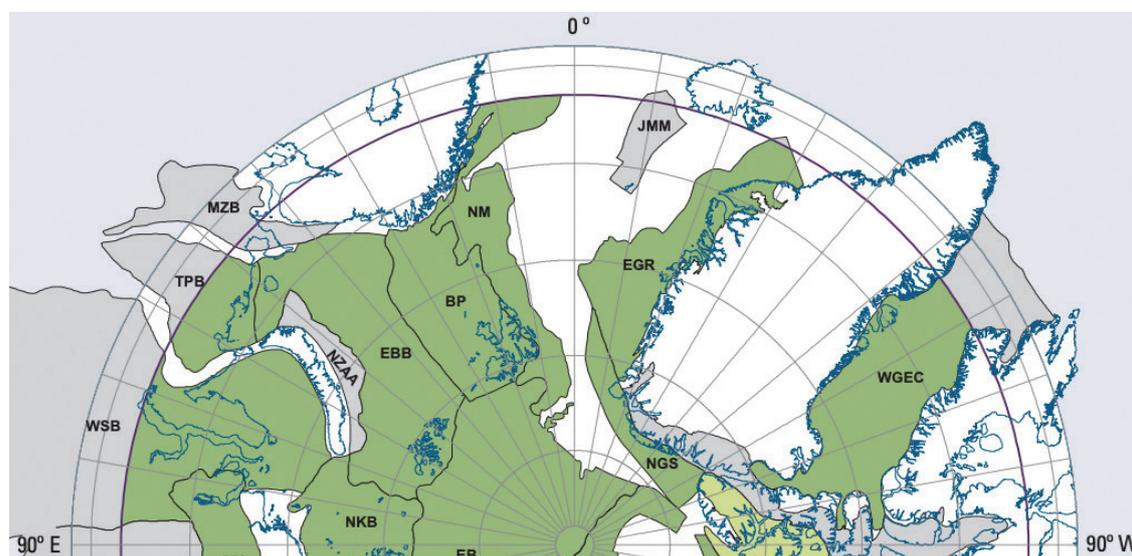


Figure 5: Areas of undiscovered oil by province in the Arctic. NM and BP denote Norwegian Margin and Barents Platform respectively - Source: USGS

BEYOND THE CIRCLE

Canada, Russia, Denmark, Norway and the US aren't the only nations interested in the Arctic. Despite its distance from the region, the People's Republic of China became an observer to the Arctic Council in 2013 and is another cause of the rising tensions in the region. China has self-defined itself as a 'near-Arctic state' based on the impact of climate change in the Arctic on China and more recently on the assertion of China's rights and interests in the Arctic under international law. In 2018 the nation published its first Arctic Policy which outlined its plans to increase its activity in the Arctic in order to gain its own share of the resources while also setting out President Xi Jinping's concept of building 'a community with a shared future for mankind'. At the time of writing, China has not expressed an opinion on the extended continental shelf claims submitted to CLCS. It is however extremely interested in maritime space in the Arctic Ocean being considered as international waters and seabed, where they would have the same rights as Arctic states and enable them 'lawful and rational use of Arctic natural resources' in China's words (though it remains to be seen what that will mean).²⁹ China's other main interests in the Arctic include advancing scientific research for strategic purposes which is required to enhance the country's shipping and resource extraction ambitions, harvesting fish in the mid to long-term as fish stocks move northwards due to warming seas and introducing security, insurance and rescue systems for development of Arctic tourism. The Northern Sea Route, called by the Chinese the Polar Silk Road, is also prioritized in their Arctic policy. This comes back to the importance of new shipping routes in the Arctic, which are much shorter and safer saving money and time.

The European Union has been another party with a large interest in the Arctic. Like China, the EU's Arctic policy includes sustainable development and climate change issues. It differs from their policy with their third objective to engage in cooperation on Arctic matters at all levels³⁰ however, and its attempts to have greater influence on the region have been thwarted. The EU's application in 2009 was blocked by Canada, the chair of the Arctic council at the time, in response to the EU's ban on commercial seal product trading³¹, affecting the livelihoods of Canada's northerners and Arctic indigenous populations. It was branded an "offensive bit of unfair interference by arrogant southerners in the lifestyle of the Canadian people [and] a huge, huge issue" by the indigenous Canadian leader of the council at the time Leona Aglukkaq³². The European Parliament only worsened their



Members of China's National Arctic Research Expedition set up an ocean profiling float near the "Snow Dragon" icebreaker - Source: Xinhua News Agency

standpoint when they proposed an international Arctic Treaty, similar to the Antarctic Treaty, that was flatly denied by the Arctic states as they viewed it as a threat to their sovereignty to the region. China, Japan, South Korea, Singapore, India and Italy were all accepted as observer states under the new criteria in 2013 and welcomed to the Arctic table but the EU was not, still due to the seal ban issue. Since 2013 the Arctic Council accepting the EU's request has become more and more unlikely as deliberation has come at the expense of making progress on the council's objectives and the EU's deteriorating relationship with Russia will make it difficult to achieve a consensus. On the other hand, China has used investment and trade to gain a greater influence in the Arctic, particularly economic leverage over vulnerable Arctic states. Chinese foreign direct investment totalled \$2 billion in Greenland and \$1.2 billion in Iceland according to a 2017 CNA report.³³ The Icelandic investment accounted for almost 6% of the nation's gross GDP for the 5 year period observed by the CNA report, and consequently has made Iceland economically dependent on the Chinese as well as providing China access to senior politicians and influence on the nation. Though it has been more successful at achieving greater influence on the Arctic than the EU, China's practices are questionable and given the existing tensions in the region another superpower will only increase complexity in the future.



A Royal Marines Viking ATV conducts snow and ice training on Exercise Cold Response 2020 - Crown Copyright



A MILITARY RESPONSE

RUSSIA

In response to the rising tensions over resources and territory, the Arctic States and NATO have increased their military activity in the region. Russia has shown the greatest increase in military presence in the last decade; as well as re-establishing its Soviet Arctic infrastructure and building more airfields and naval ports from scratch, last year it doubled the number of times it entered US airspace with long-range bombers and fighter jets³⁴ and in late April 2020 a task force of Russian paratroopers conducted the first ever high-altitude (33000ft) jump into the Arctic. Since 2014, 14 airfields have been opened and there are future plans to build more airstrips for their supersonic MIG-31 jets and long-range Bear bombers³⁵. Many more of the new facilities along the Russian coast house air defence mechanisms, anti-aircraft weapons and radar systems to warn of incoming attack and to protect Russia's new 'cold' front. Patrols by long-range strategic bombers recommenced in August 2007 for the first time since the end of the Cold War and since 2017 Russia has been routinely simulating mock air attacks on Norwegian military assets³⁶. According to official sources, the Northern Fleet (Russia's Arctic naval fleet) conducted more than 100 patrols over the Arctic Ocean in 2018³⁷ and it has seen a major modernisation in the last ten years after a long period of neglect following the Soviet era. The fleet has 39 warships and 42 submarines - more than half of Russia's entire submarine fleet. Russian troops have been permanently deployed in the Arctic since 2013 and numbers of personnel range from a battalion (500-700 troops) for a small base to a brigade (3000+ troops) for the largest bases. It is hard to forget the beluga whale found off the north Norwegian coast in April 2019 that had a Russian alleged 'spy system' attached to it by a harness³⁸. The whale was found with a GoPro attachment but no camera just over 400km away from Murmansk where Russia's Northern Fleet is based.

While Russian officials and its Ministry of Defence have declared these new bases and installations serve the purpose of securing the Northern Sea Route, the world remains sceptical. The radars are designed to identify and track airborne targets – not surface ships – and it is difficult to justify dangerous high-altitude parachute jumps to protect vessels sailing through the Northern Sea Route. What this activity is most likely to be about is 'showing its muscles' to the rest of the Arctic States (especially to the smaller nations of Denmark and Norway), NATO and the rest of the world to demonstrate its commitment and determination to display sovereignty. In addition, Russia's military puts defence of the Kola Peninsula as a priority to secure the nuclear assets there and the access of its Northern Fleet, and as such the peninsula is seen as of enormous strategic importance for Russian national security. The Kola nuclear complex is Soviet era, but today the region has extended towards the Barents Sea and Norwegian Sea as part of a 'bastion concept'.³⁹ As natural gas and oil facilities are seen as strategic assets for Russia, they are being increasingly factored into the concept as well.

USA

The US is another major military player in the Arctic as it is around the world and like Russia has been increasing its military activity there. Despite their views on climate change, the Trump administration adopted a more prominent military presence in the region than in years

before when focus was on the Middle East and Afghanistan which included an updated Arctic Strategy paper. The US Department of Defence outlined 3 objectives in the paper; 'defending the homeland'; 'compete when necessary to maintain favourable regional balances of power'; and 'ensure common domains remain free and open'.⁴⁰ In order to achieve these goals, the US Coast Guard will receive new desperately required icebreakers as its single, ageing icebreaker poses a huge weakness to the US's military presence in the Arctic because it limits military, commercial and search and rescue operational capabilities. Russia, on the other hand, has the largest icebreaker fleet in the world. The US will also begin conducting 'freedom of navigation operations' to contest Russia's claim that the Northern Sea Route is not international waters. The 3 US bases in the Arctic from which they conduct air defence operations, Thule Air Base in Greenland, Joint Base Elmendorf-Richardson in Anchorage, Alaska and Eielson AFB in Fairbanks, Alaska, have received huge infrastructure investments as part of the 2019 US Arctic Strategy. This has included increasing the number of advanced aircraft in the region including a new squadron of the cutting-edge F-35A Lightning II fighter jet for AFB Eielson⁴¹ as part of a \$500 million investment into the base which also included the addition of 1300 personnel, twice the number of personnel stationed at the airfield before⁴². Also at Eielson AFB is a fighter wing dedicated to acting as the 'aggressors' or 'enemy' for combat exercises - often replicating Chinese and Russian tactics in aircraft painted in their patterns and colours to sharpen the USAF's dogfighting capabilities⁴³.



a F-35A Lightning II assigned to the 356th Fighter Squadron lands at Eielson AFB, Alaska, June 25, 2020. Source: USAF



a USAF F-16 from Eielson's 18th Aggressor Squadron painted in a Russian style blue and grey pattern Source: USAF



NATO

Of the 8 Arctic States, all but Russia are members or partner countries of NATO. The Arctic was top of NATO's security agenda during the Cold War as the nuclear missiles would have come over the North Pole and Russia's Northern Fleet is based there. However, after the collapse of the Soviet Union, its significance was reduced until climate change's impact on the region reignited tensions and redirected attention.

NATO has stated its main security concern in the Arctic has been the rapid build-up of Russian military there since 2008 as part of a wider problem of Russia's military modernisation. In addition, Russia's military aggression in other parts of the world including Crimea has raised concerns over further regional instability and conflict. Exercises Cold Response, Dynamic Mongoose and Arctic Challenge are the heart of NATO's military activity in the Arctic and in 2018 Norway hosted Exercise Trident Juncture. This biennial exercise is a NATO-led joint force exercise to ensure NATO forces are trained and ready to work collectively in different environments, usually those of particular concern or instability at the time. The 2018 exercise took place in central and eastern Norway and the surrounding areas of the North Atlantic and the Baltic Sea, including Iceland and the airspace of Finland and Sweden. Air, land, maritime, special and amphibious forces of 31 NATO and partner countries participated, involving around 50000 personnel, 250 aircraft, 65 vessels and 10000 vehicles⁴⁴ making Trident Juncture 2018 one of the largest military exercises ever held in Europe and the largest conducted by NATO for decades. Despite this, NATO regularly states that while it is a defensive exercise it is not directed against any country, although given its view of similar Russian exercises as threatening, it would be reasonable for Russia to justify seeing it the other way around. Exercise Cold Response is a major Norway-led military exercise that has taken place biennially since 2006. It is designed to boost the abilities of soldiers across NATO operating together in extreme cold weather conditions⁴⁵. The UK has been a key participant in the exercise since it began, with 1250 Royal Marines and four Royal Navy and Royal Fleet Auxiliary ships taking part in 2020 making the UK the largest contributing nation in terms of personnel besides Norway.

CHINA

China's involvement in the Arctic has raised concerns for NATO and the US over whether they will

begin military activity in the future and whether they will be a future threat to arctic security and stability. With no military plans included in China's 2018 Arctic policy or any official statements on its military intentions in the Arctic, it has made it even harder for NATO to predict what China will do next. It is known China has outpaced the US in construction of icebreakers and China's military has been using the scientific knowledge it has collected in the Arctic, its relationship with Russia and investment in Greenland and Iceland as a way into the region. In 2016 China's attempt to purchase an old military base in Greenland was stopped by Denmark under US guidance and in 2018 the US also advised Denmark to reject a blacklisted Chinese company's offers to construct international airports there too⁴⁶. In a CNBC interview in August 2019, the NATO Secretary-General Jens Stoltenberg stated "we need to assess the security consequences, for all of us, of the rising military power of China" in the context of China's military presence in the Arctic, and also that the "alliance is carefully

monitoring China's increased physical presence [in the Arctic]"⁴⁷. While China's military has not made any significant moves in the Arctic yet, it is important to consider its activities in the South China Sea which are also over resources and shipping routes. Since 2013, China has built a handful of islands in the South China Sea with runways, military bases and anti-ship, missile and air defences on them to intimidate the six surrounding states and thereby gain greater influence in the region as part of its efforts to claim a 2 million sq. km area of the sea. Tensions have regularly spiked between the US and China in the South China Sea including on 9 May 2020 when China took advantage of the global Covid-19 pandemic to mount a display of military firepower, immediately triggering a rapid response from Washington to send three warships to the region.⁴⁸ China's activity in the South China Sea demonstrates China's aggressive tactics and its willingness to take on the US which it could bring with it into the Arctic.



HMS Kent in the icy Barents Sea, May 2017 – Crown Copyright

PEACE OR CONFLICT?

The Svalbard Archipelago is a rocky, isolated and unique set of islands between Norway and the North Pole (see figure 1). While it has been part of the Kingdom of Norway since 1925, Svalbard is not administratively part of Norway, the Schengen Area nor the European Economic Area. The Svalbard Treaty⁴⁹, effective since 1925, recognizes not only the sovereignty of Norway over the islands but also regulates demilitarization of the region, gives the 46 signatories equal rights to economic activities on the islands and creates a visa and tax-free zone. The need for the treaty of such a desolate and distant place originally became necessary as mineral deposits including coal and oil were found on the island at the beginning of the 20th century⁵⁰, though



it displayed its enormous strategic and military importance during the Second World War when it was occupied by the Nazis. Since then, only Russia (at the time the Soviet Union) and Norway have exercised the treaty with coal mining and more recently tourism. However, as the Arctic ice sheet retreats, Svalbard is becoming even more valuable strategically and economically as it has the potential to serve as a hub of mineral extraction and shipping.

Svalbard offers a case for cooperation and peace in the Arctic because, despite the Cold War and the emerging significance of the archipelago, all signatories have respected the treaty since 1925 (with the exception of Nazi and Norwegian troops during the Second World War). The Global Seed Vault⁵¹ is located here because of the stability of the islands as well as the cold conditions, and no military equipment, buildings or personnel have been stationed here by either side despite the strategic significance of the islands to Russia and its Northern Fleet. The sustained coal mining, oil and fishing activities around Svalbard have also demonstrated their cooperation. Consequently, a similar treaty for the Arctic could be effective and prevent conflict in the region. Cooperation in the Arctic since the formation of the Arctic Council in 1996 has never been stronger with projects, initiatives and treaties, such as the Protection of the Arctic Marine Environment and the Indigenous Peoples' Secretariat to name a few, which have been successful with their objectives and included support from all member states and many observer states. A treaty similar to the 1925 Svalbard Treaty with demilitarisation across the Arctic as well as equal rights for all signatories to economic activity there including oil extraction and shipping could stabilise the region and therefore could be an effective and appropriate means of de-escalating tensions in the Arctic.

However, not only would a treaty like this be very difficult to implement as the Arctic States would want to defend their borders and keep resources to themselves but also the Arctic Council does not have the mandate for peace and security concerns so, while its environmental and sociological programmes have been successful, its lack of power prevents it from creating a treaty like this. Although the rising tensions in the Arctic have caused a reconsideration of the council's role in geopolitics and security affairs, the economic and strategic objectives of the member states would make introducing these powers unlikely because all the decisions of the council and its members are taken by consensus. Besides, a treaty such as this would be created by the United Nations and not the Arctic Council, as the majority of the Arctic is still international waters under the UNCLOS and also it would fall under the United Nations' central mission for the maintenance of international peace and security. Were the UN to create a treaty for maintaining peace and security in the Arctic, the lengthy-time lag for a treaty on this scale to be written, agreed upon and signed would give the Arctic States plenty of time to agree on their borders between themselves, especially since a UN treaty could give states beyond the Arctic Circle powers in and access to the Arctic region therefore threatening and impeding upon their ambitions. For example, the 2017 Paris Agreement on greenhouse-gas-emissions mitigation, one of the most recent and largest UN treaties, took 12 years to become effective which was based upon the 2005 Kyoto Protocol which in turn was an extension of the 1992 United Nations Framework Convention on Climate Change⁵². A new treaty, therefore, would take a minimum of 10 years to be written, signed and ratified which would give enough time for the Arctic States to agree upon a deal between themselves.

This time lag for a UN treaty would also be too slow because the size of the Arctic ice sheet is decreasing so rapidly that new resources and shipping routes are becoming accessible all the time and consequently pressure on the Arctic States has increased as the ice sheet has melted to not only protect the Arctic from further environmental damage but also to agree to cooperate in order to safely and peacefully obtain as much wealth and strategic power in the region as they can. Their extended continental shelf submissions are an example of this because all the Arctic States followed UN protocol rather than simply declaring that the territory was theirs and using naval force to defend it - it is only because of the UN's decision for conflicting claims to be agreed upon between the Arctic States themselves that tensions have arisen. Russia, Canada, Denmark and Norway are huge beneficiaries of the United Nations Convention on the Law of the Sea and so are unlikely to disregard it, although the dispute over the Barents Sea between Russia and Norway took over four decades to be agreed upon⁵³ and an agreement between Russia, Canada, Denmark, Norway and the US could take even longer because the delimitation of the Barents Sea was only a dispute between two nations.

None of the Arctic States has been as assertive and impatient as Russia in the competition for resources. Oil and gas are a pillar of their economy, accounting for 60% of Russia's exports and 30% of the nation's GDP⁵⁴. A country with an economy built on oil and gas needs to exploit the Arctic's resources as far as it can, especially since it has struggled with a stagnating economy and depleting inland reserves in the past few years. GDP growth in 2019 was just 0.5%, underperforming all estimates, and Russia has a GDP per capita lower than Greece. Their increased military presence in the Arctic is most likely to protect their Arctic economic activities but Russia's controversial actions toward other Arctic states, such as intrusion upon US airspace and mock air attacks on Norway, not only is a tactic they are using to assert dominance in the Arctic but also demonstrates they are willing and ready to fight in order to protect their Arctic activities, therefore bringing the risk of conflict to the region. The US and NATO's response to this has been to increase their military presence in the region, conducting enormous military exercises and improving their Arctic defence systems in order to protect their Arctic activities from what they perceive as a threat from Russia. This suggests the relationship between NATO and Russia is a peaceful standoff because both sides are acting defensively with neither seeking to invade or interfere with each other's activities in the Arctic region. It does not suggest cold warfare, however - cold warfare is conflict pursued primarily through economic and political actions, espionage and proxy warfare as used in the US-USSR Cold War and also arguably the ongoing tensions between Pakistan and India.

Nevertheless, the conflict in Ukraine since 2014 and the annexation of Crimea points towards an aggressive and forceful Russia which establishes concerns for conflict in the Arctic. In 2014 Russia carried out a takeover of Crimea using unmarked military personnel then dismantled the government forcing a referendum on whether Crimea should become a part of Russia. This referendum was ultimately dubbed a 'gun-point' referendum and recognized invalid, causing more unrest in the region. Meanwhile, in Eastern Ukraine, a ceasefire and security zone was put in place in 2015 after a year of deadly fighting between Ukrainian and Russian-backed separatists forces, though it has been broken many times since. Almost 10000 people have died in the





Ukrainian soldiers in the eastern security zone, 2015
Source: Telegraph

conflict and over 1.5 million have been displaced⁵⁵. Although the primary explanation given for why this conflict has happened is the almost even split between pro-EU and pro-Russia voters in Ukraine, there is also strategic importance to the region and a large oil and natural gas presence. The port of Sevastopol in Crimea was the base of Russia's Black Sea fleet during the Soviet Era, important for access to Georgia, the Middle East and North Africa, and there are large volumes of oil and gas deposits in the Black Sea. The similarity to their reasons for entering the Arctic and the relatively small size and sparse population of some Arctic States such as Norway and Greenland suggest Russia would carry out a hostile invasion of territory in the Arctic in order to obtain oil and gas and ensure its strategic and economic security. This is even more likely when there would be no civilian resistance as there is in Ukraine so Russia would be able to deploy their soldiers to full operational capability with all equipment and vehicles which they weren't able to do in Ukraine. The demonstration of force in Ukraine by Russia gives enough justification for NATO's concern for conflict in the Arctic and threatens the stability and peace of the region.

Furthermore, China's activities in the South China Sea could present a threat to Arctic security too if China were to work with Russia economically and strategically. The South China Sea conflict is a territorial dispute with a resemblance to the Arctic tensions; the objective in the South China Sea is obtaining oil, natural gas, fishing and shipping routes but territorial claims are being disputed or have been denied. Although not as violent and confrontational as the Ukrainian crisis, China's intense military activity in the South China Sea also offers reason for conflict in the Arctic, particularly if the working relationship between Russia and China in the Arctic continues. NATO has responded to the unrest in the South China Sea but to a lesser extent than in the Arctic, although two US aircraft carriers were sent to the region as recently from writing as June 17 2020⁵⁶ and HMS Queen Elizabeth's first operational deployment will be there too. In addition, the fragile tensions between China and the US over trade and coronavirus have resulted in increased military activity on both sides, particularly in the South China Sea. In response to questioning by China on why they are operating in the region, the US has stated it is practising its right of free passage and navigation, though it is evident that is not the case. The US most likely has its own interests there, most of all the free travel of ships from China to the west as a third of the world's shipping passes through the South China Sea and also to protect its allies in the region including Japan, Philippines and Vietnam. Both the confrontation between the US and China and China's military actions in

the South China Sea display a willingness for using military force and if China were to continue working with Russia to obtain its own share of resources and shipping routes especially since the Northern Sea Route has enormous potential, Russia, China and the US could pose a significant threat to Arctic stability and cause for conflict in the region.

In addition, the US has a history of fighting for oil and so, while the US sees Russia and China as a threat to Arctic stability, the same could be the other way around. The Iraq War, for example, had highly questionable motives with the former head of U.S. Central Command and Military Operations in Iraq, General John Abizaid, saying "Of course it's about oil; we can't really deny that," in 2007. The Iraq War was far more violent and direct than the Ukraine Crisis has been so far as well. Despite an abundance of oil in the United States mainland, the US still chose to invade Iraq with the ulterior motive to be able to drill for oil in its rich oil fields. Why they did this may have been to ensure it has control of the world's oil supply and therefore maintain stable and reasonable global prices for it in a region of prior instability or was wealth led with US trans-national corporations utilising the fields for themselves. With the invasion's UN-backing it is more likely to have been the first reason, but the second is still plausible as a secondary motive for the US. The Arctic's instability and the potential for enormous resource wealth there are similar to the most likely motives of the Iraq invasion but the fact that the US has not ratified the UNCLOS and as such is unable to make a claim to the oil and gas rich Arctic Alaska region will make it difficult to prevent foreign oil companies including Chinese and Russian drilling there if the Arctic Ocean remains international waters. Consequently, the US may use naval force to deter foreign interest in the region and, as it is in the South China Sea, conduct 'freedom of navigation' operations to show its military strength and willingness to fight if necessary. There is also the case for strengthening national security; it is important for a country to be able to supply itself with food, water and fuel for a length of time if foreign imports are cut off and therefore the US may be interested in exploiting the Arctic Alaska resources before it exploits its mainland reserves, which it would use in a situation such as this. Take the purchasing of most of the world's supply of remdesivir, a drug that reduces recovery times for Covid-19 patients, as an incredibly recent example of the US protecting its national security through the control and supply of resources⁵⁷. Subsequently, not only are Russia and China risks to conflict and instability in the Arctic, but the US also is as much of a risk, if not greater than, because of its national security interests and history with oil wars which could cause tensions to escalate in the Arctic between the three nations.

A conflict between Russia, China and the US in the Arctic in the form of global warfare is incredibly unlikely, however, because the mass-destruction, expense and loss of life that would come with it means they are avoiding it at all costs. The Cold War, it could be argued, never escalated into a confrontation because the world did not want to relive the consequences of global warfare after the First and Second World Wars. There were enough incredibly close calls that could have triggered either the Americans or Russians to react⁵⁸ but they never did. The January 2020 standoff between Iran and the USA after the assassination of General Qassim Soleimani is a more recent example of limited but intense confrontation because both sides adamantly want to avoid conflict, and the rest of the world's reaction seemed to be the same with nations including the UK calling for "urgent de-escalation".



Instead of global warfare, nations have begun to fight through proxy warfare in the last 30 to 40 years, which is when two factions receive indirect support from other nations usually with similar or the same interests. Proxy warfare enables the proxies to fight other nations and governments while avoiding the disastrous effects of global warfare and was a characteristic of the US-USSR Cold War. Furthermore, the almost immediate declaration of America and Iran after the killing of General Qassim Soleimani that they would prefer proxy wars instead of direct conflict and the expectation that Iran will avenge the US by using its proxy network⁵⁹ demonstrates the present use of proxy warfare as a way of avoiding global warfare. However, the sparse, small and content indigenous population of the Arctic means there would be no factions for the nations to fight through and so a proxy war in the Arctic would not be possible. Therefore, conflict in the Arctic is unlikely if the nations are not willing to use conventional and global warfare instead and so peace seems more probable.

Additionally, the responses to conflicts such as NATO's to the Ukraine Crisis demonstrates not only the shift away from global warfare but also another reason for no conflict in the region. The reaction by NATO to the Russian invasion of Ukraine was incredibly slow and, although Russian soldiers were using unmarked uniforms making it harder for them to identify the force, there has been very little response or support by NATO to Ukraine since the crisis began other than sanctions on Russia by the US and EU. These sanctions seem to have had little impact on Russia as the crisis is ongoing. This NATO reaction gives the impression that Russia would be sanctioned in response to an invasion of territory in the Arctic and so not only would this encourage Russia to carry such an action out if the economic value of the Arctic is greater than the sanctions imposed but also suggests peace in the region given that NATO would not respond forcefully. Additionally, President Putin may have used his invasion of Ukraine as a 'test' of NATO's response, just like Russian aircraft regularly enter US and NATO airspace with fighter jets and bombers to test reaction speed, but this is difficult to verify. Moreover, US-China tensions have resulted in sanctions rather than conflict indicating the same approach from the US and China outside NATO and therefore further indicates the use of sanctions rather than force in this situation in the Arctic. However, Putin cannot rely on NATO's response to the Ukraine Crisis to be the same if he were to invade elsewhere because Ukraine is not a member of NATO and so NATO was not obliged to respond. An attack on Norway, Canada, Denmark or the US, on the other hand, would trigger a NATO reaction according to Article 5 of the Washington Treaty - 'an attack on one member is an attack on all'. Article 5 was triggered following the 9/11 attacks on the USA initiating the 'War on Terror' but otherwise has not been used, signifying the extremity of an action that would result in it. Russia is the only Arctic State not in NATO and so it would be dangerous for Russia to invade or attack another nation's territory in the Arctic because, unlike in Ukraine, a NATO military response would be almost certain and so peace and security in the region are likely to remain stable.

Nonetheless, with the emergence of hybrid warfare, it has become more difficult for NATO and other countries to justify a large-scale military response and so Russia could assert itself in the Arctic without triggering Article 5. Hybrid warfare is a blend of political warfare with other influencing and conventional methods and has seen a large increase in use in the 21st century. Since 2010 the number of



9/11 Attacks - Source: AFP / Seth McAllister

occurrences of hybrid warfare have increased and have been between large nations such as the ongoing Indo-Pakistani Kashmir conflict or USARussia activities. Utilising fake news, electoral intervention and creating a lack of legitimate targets are just a few examples of the subversive nature of hybrid warfare. Unlike the 9/11 attacks which were characterised by their clear aggression toward the US by a specific group, hybrid warfare's elusive nature makes it harder to target an individual, organisation, state or faction and therefore justify and plan a response to the threat. In addition, cyberwarfare is even harder to combat because it is even more obscure than hybrid warfare yet it can be used to cause enormous destruction non-violently⁶⁰ - creating nation-wide power outages, cutting phone lines and paralyzing infrastructure are no longer science-fiction⁶¹ for example as Ukraine has experienced all these cyber warfare tactics in the last few years as part of Russia's use of hybrid warfare in the crisis which has also included the manipulated referendum, fake pro-Russia and anti-EU news and the use of a conventional fighting force in the invasion of the country. Consequently, a conflict between the Arctic States for territory in the Arctic may not be fought there. Instead, it could take the form of hybrid warfare, using political, cyber and conventional warfare techniques. This may look like targeted cyber-attacks on radar systems between the US and Russia, disruption of Norwegian infrastructure projects, or political intervention by China in Greenland for example which are hard to identify a target for or justify an aggressive nature and thus makes it more difficult to respond to. Therefore, conflict over resources and strategic power in the Arctic may be concealed by a non-violent cyber, political and unconventional conflict beyond the region and so suggests neither peace nor conflict.

CONCLUSION

With little evidence of cooperation between the Arctic States over the territorial claims, the tensions look set to continue. Whether these tensions escalate into conflict or turn to peace and cooperation relies on the Arctic States coming to an agreement between themselves over territory, resources, shipping routes and the environmental protection



of the Arctic if they wish to maximise the economic and strategic opportunity in the region peacefully, sustainably and legitimately. If they do not, the Arctic States risk losing exclusivity to these opportunities and therefore will not be able to achieve all of the economic and strategic potentials the region holds as well as risk an escalation into conflict. Russia's economic situation means expansion into the Arctic to increase its oil and gas supply is one of the only options for stabilising and growing its economy and so cooperation should be a priority for them. Another, one could argue, was the invasion of Ukraine and annexation of Crimea in order to access the resources in the Black Sea but as identified the success of a similar operation in the Arctic is very unlikely. If no agreement is made, of all the Arctic States Russia is, therefore, most likely to escalate the tensions in the region. On the other hand, Canada and the US are less likely to be part of the economic race in the Arctic because of the abundance of oil and gas reserves in their own countries which are cheaper and easier to access, however, the US has demonstrated strong interest in protecting Arctic Alaska and they see Russia as well as China's interests in the Arctic as a threat to their national security and the security of the Arctic. If the Arctic States want to not only maximise the economic and strategic opportunities of the Arctic but also stabilise the region they have to agree on territorial boundaries. While this is would currently be difficult to do, if the Arctic Council were to have a mandate for peace and security concerns then a platform would be created for the Arctic States and observer states to agree upon these issues and therefore prevent conflict in the region. Therefore, a peaceful agreement or a mandate for the Arctic Council to have power over peace and security concerns is vital for calming tensions in the Arctic Circle.

If an agreement is not made however, then conflict is a possibility. Conflict for resources in the Arctic could take several forms. Firstly, the NATO-Russia standoff in the Arctic could remain and so while the tensions would continue there would be little to no confrontation. NATO members including the UK and the US would continue to train in the Arctic not only to prepare for a conflict if tensions were to escalate further but also to show Russia and China that they are actively defending and willing to combat potential threats to Arctic security and their own national security. Meanwhile Russia would also continue to exercise and demonstrate force against NATO in the Arctic but overall neither side would seek to confront one another. Therefore, while not peaceful, conflict in the region could be non-confrontational standoff between the two sides of the Arctic. It is important to reiterate however that this would not be cold warfare. Alternatively, if Russia were to invade Norwegian territory with its military or China were to make an aggressive move upon the US Air Force base in Greenland in the future then Article 5 could be triggered, and NATO would have to respond to the threat. How severe a threat this is would determine the extent of the response –if the Russian mock air attacks on Norwegian assets practiced by them since 2017 became for real it would trigger a more aggressive and larger response than Chinese interference in a Greenlandic election, for example. NATO already has in place a strategy for a response to an attack from Russia such as this and Exercise Trident Juncture was one of many practices of it. A war between NATO and Russia utilising global warfare in this scenario would be catastrophic, however, which is why of all conflict scenarios it is the least likely as all nations wish to avoid it.

A hybrid war, on the other hand, is more likely if tensions escalated.

huge scope for hybrid warfare in a conflict for resources in the Arctic makes it even more difficult to predict what the new 'cold' war in the Arctic will look like and to what extent will it be violent, although its subversive nature makes it a very likely way in which conflict in the region could be fought. Most likely, however, is that conflict in the Arctic is fought outside the Arctic Circle. As identified proxy warfare in the Arctic would not be possible however existing proxy wars could be where the conflict for resources in the Arctic is fought instead. For example, in a situation where Russia were to conduct a cyber-attack against Norway, the US could respond by supplying weapons to the Combined Joint Task Forcebacked Rojava or conduct a series of airstrikes against the Russian-backed Hezbollah in the Syrian Civil War. Not only would this take the conflict outside of the Arctic, but also prevent the consequences of a violent conflict between NATO and the US which is why it is the most likely of all the possible conflicts if no agreement over territory and resources can be made.

Ultimately conflict in the Arctic would be the last resort for when no agreement can be made and the Arctic States see a threat to their nation's security or desperately require Arctic dominance for the prosperity of their economy, as in the case of Russia. The lack of cooperation suggests conflict is on the horizon, and while war outside the Arctic is the most likely it is nearly impossible to predict how exactly the conflict will look like as with many other regions of tension around the world including the South China Sea and Kashmir. All in all, one can only hope the Arctic States come to an agreement over territory in the Arctic Circle and tensions calm to prevent the new 'cold' war.



*A member of 30 Commando Information Exploitation Group Royal Marines on a skidoo during Exercise Cold Response at the beginning of 2020
Front Cover of the Globe and Laurel March 2020*

Source: Royal Marines



Can you ever truly mix a cuppa? Spilling the tea on Brouwer's Fixed Point Theorem

Ben Watkins

INTRODUCTION

Is it possible that there are always two places on earth with the same temperature and pressure? How does the game show Blockbusters have any implications on algebraic topology? Can a general equilibrium ever be reached in an economy? Perhaps most crucially of all, can you ever truly mix a cup of tea?

My IIA provides insight into Brouwer's fixed point theorem, a theorem found in the field of algebraic topology. It uncovers how a remarkable and seemingly counterintuitive result in what is often considered to be an abstract field of mathematics can have such broad and pertinent results in the real world. However, this isn't to say that this IIA doesn't uncover the result of this theorem for the sake of the beauty of it as much as uncovering it for the sake of its applications. Indeed, Luitzen Egbertus Jan Brouwer himself (the discoverer of this theorem as well as often being called 'the Father of Topology') was very much an upholder of this mentality: that maths has great importance for the sake of maths itself. Philosophically, Brouwer was a neo-intuitionist, which means that he thought of mathematics as purely a mental phenomenon, the result of constructive mental activity rather than uncovering any principles of an objective reality. He is often quoted in saying that "The construction itself is an art, its application to the world an evil parasite."

WHAT IS BROUWER'S FIXED POINT THEOREM?:

The Brouwer's Fixed Point Theorem states that given a compact and convex set α that is the subset of some Euclidean space \mathbb{R}^n for any value of $n \geq 1$, we can apply any continuous function f and there will always be some element, $c \in \alpha$ such that $f(c) = c$. Convex here means that for x, y in X , $cx + (1-c)y$ belongs to X for any $0 \leq c \leq 1$ i.e. given any two points that exist within the set, any point that exists along the line segment which connects these two points must also be a member of the set. Compact here means that all points within a set lie within some fixed distance of each other and that all the sets' limit points are self-contained within the set.

In simpler terms, what this theorem says that suppose that we have some object. Now, imagine this object as being made up by an infinite amount of points within the object. This object is bounded and doesn't have any holes in it. Now say that we can mould this object by stretching it, crumpling it, twisting it, and bending it but we aren't allowed to tear it or glue it. What Brouwer's fixed point theorem states is that at least one of those points within the object will stay in the same place that it started in, no matter how much we try.

For example, take two pieces of paper, leave one flat but take the other

and crumple it as much as you desire and then place the crumpled piece of paper on top of the flat piece of paper. By Brouwer's fixed point theorem, we can say with certainty that at least one point of that crumpled piece of paper is directly above the point on the flat piece of paper that it would've been if we hadn't crumpled the piece of paper in the first place. The theorem doesn't say exactly where this point is but simply, that there is one.

The first part of my IIA shall cover how we can go about proving this to be true in both the 1-dimensional case and in the 2-dimensional case of a closed and bounded disk embedded in the \mathbb{R}^2 space. Then afterwards, I will delve into both major applications of this theorem for us in the real world as well as ending on some more trivial and novel facts that come about as a result of this theorem.

1 DIMENSIONAL PROOF:

THIS PROOF COMES IN THREE STAGES:

1. Proving *Image of Interval by Continuous Function is Interval*
2. Proving *Intermediate Value Theorem*
3. Proving *Brouwer's Fixed Point Theorem in 1 dimension*

1. PROVING IMAGE OF INTERVAL BY CONTINUOUS FUNCTION IS INTERVAL

Theorem: Let I be a real interval. (A real interval is a range of numbers between two given numbers and includes all of the real numbers between those two numbers.)

Let $f: I \rightarrow \mathbb{R}$ be a continuous Real Function. (A continuous function is a function that does not have any abrupt changes in value such as in $y = 1/x$ for example)

Then the image of f is a real interval (an image of a function is the set of all output values it may produce)

Proof: Let J be the image of f .

Suppose that we have two points $y_1, y_2 \in J$, and suppose that $\lambda \in \mathbb{R}$ where $y_1 \leq \lambda \leq y_2$.

Let $S = \{x \in I : f(x) \leq \lambda\}$ be the subset of the interval I where $f(x)$ is less than or equal to λ

Let $T = \{x \in I : f(x) \geq \lambda\}$ be the subset of the interval I where $f(x)$ is greater than or equal to λ



As $y_1 \in S$ and $y_2 \in T$, it suffices to say that $S, T \neq \emptyset$.

Also, $I = S \cup T$.

Let $s \in S$ be a point that is at zero distance from T . Such a point can exist as S and T are both closed and share a boundary.

Let $\langle t_n \rangle$ be a sequence in T such that:

$\lim_{n \rightarrow \infty} (t_n) = s$. (the proof of the possibility of this is excluded but it is shown to be true by the 'Limit of Sequence to Zero Distance Point Theorem')

Since f is continuous $I: \lim_{n \rightarrow \infty} (f(t_n)) = f(s)$.

But for all $n \in \mathbb{Z}^+ : f(t_n) \geq \lambda$. Hence we have that $f(s) \geq \lambda$.

But because $s \in S$, we have that $f(s) \leq \lambda$, as per our definition of S .

Therefore $f(s) = \lambda$ and so $\lambda \in J$.

(NB: the same can be done by considering a point t at zero distance from S .)

2) PROVING THE INTERMEDIATE VALUE THEOREM

Theorem: Let $f: S \rightarrow \mathbb{R}$ be a real function on some subset S of \mathbb{R} .

Let $I \subseteq S$ be a real closed interval of S

Let $f: I \rightarrow \mathbb{R}$ be continuous on I .

Let $a, b \in I$

Let $k \in \mathbb{R}$ lie between $f(a)$ & $f(b)$.

That is, either: $f(a) < k < f(b)$ or $f(b) < k < f(a)$.

Then $\exists c \in (a..b)$ such that $f(c) = k$

(Effectively, this theorem states that on a continuous function, if you have two values on the function, then the function must contain every value on the range of these values in between these values.)

Proof

From image on interval by continuous function is interval we know that the image of $(a..b)$ under f is also a real interval.

Thus, if k lies between $f(a)$ & $f(b)$, it must be the case that $k \in \text{img}(a..b)$.

3) PROVING BROUWER'S FIXED POINT THEOREM IN 1 DIMENSION

Theorem:

Let $f[a..b] \rightarrow [a..b]$ be a real function on the closed and compact interval $[a..b]$ and let $a > b$ (A closed interval is an interval that contains its endpoints so in this case, an interval which contains both a & b and everything real in between.) (NB any subset of Euclidean space \mathbb{R}^n , that is closed is bounded according to Heine-Borel theorem, however this is evident in our case since it can be covered by an open interval $(a - 1, b + 1)$.)

Then there exists a point $c \in [a..b]$ such that $f(c) = c$.

Proof:

As the Codomain of f is $[a..b]$, it follows that $f \subset [a..b]$ (The codomain

is the bit after the arrow in the definition of a function.)

Hence, $f(a) \leq a$ and $f(b) \geq b$. (statement 1)

Let $g: [a..b] \rightarrow \mathbb{R}$ such that $g(x) = f(x) - x$ (statement 2)

As both $f(x)$ and x are continuous functions, $g(x)$ is continuous on $[a..b]$ (This isn't a necessary given, but it is intuitive and proven by the combined sum rule for continuous functions. However, this isn't true for infinite sums of continuous functions as seen in Fourier Series, but we needn't concern ourselves.)

By combining statement 1 and statement 2, we can see that:

$g(a) \geq 0$ and $g(b) \leq 0$

Using the intermediate value theorem, by letting $k=0$,

We know that there must exist a point $c \in [a..b]$ such that $g(c) = 0$.

Therefore, as $g(c) = f(c) - c$, there must exist a point where $f(c) = c$

AN INTRODUCTION TO CATEGORIES AND FUNCTORS:

A Category in Mathematics refers to a group of objects that are linked by 'arrows' which symbolise morphisms between the objects. (A Morphism being another way to refer to a function, particularly between two different mathematical structures.)

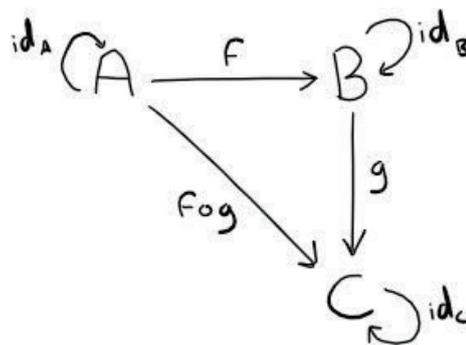
To be classed as a category, two basic criteria must be fulfilled: firstly, that arrows are associative and secondly that each object has an identity arrow, a morphism that returns itself. An example of a category is found below (Associativity is a property that given $\{G, *\}$ where G is a set and $*$ is a function, and we have that $a, b, c \in G$, then $a*(b*c) = (a*b)*c$)

Suppose then, that we have two categories K & L , a functor F is a mapping (mapping being another term for function) from K to L such that:

1) It associates every object x in K with an object $F(x)$ in L .

2) It associates each morphism in $f: A \rightarrow B$ in K a morphism $F(f): F(A) \rightarrow F(B)$ in L such that:

- i) $F(\text{Id}_x) = \text{Id}_{F(x)}$ for every object x in K
- ii) $F(g \circ f) = F(g) \circ F(f)$ for all morphisms $f: A \rightarrow B$ and $g: B \rightarrow C$.



IMPORTANT APPLICATIONS

Despite Brouwer's neo-intuitionist approach to mathematics, his theorem has been used much in applied mathematics. Particularly, my IIA will discuss its impact on Economics and Game Theory.

ECONOMICS

Firstly, in economics, Brouwer's fixed point theorem has been used in the field of *General Equilibrium Theory*. Equilibrium in economics refers to the balance of supply and demand. Whilst partial equilibrium theory takes only into consideration a part of the market, typically single markets, *general equilibrium* considers the totality of the economy where there are several interacting markets and seeks to prove that eventually, supply and demand resolve to an equilibrium. Historically, this theory dates to the 1870s work of French mathematician Léon Walras 'Elements of Pure Economics' and his theory holds crucial importance to modern-day economies.

General Equilibrium, if achieved would be an economic utopia. It has been repeatedly shown that economies become increasingly stable the closer that they come to a general equilibrium. General equilibrium leads to the stability of prices. As prices become more stable, this means that both businesses and consumers can make long-term financial plans. This is a good position that any economy would like to be in.

The problem that we are concerned with, however, is whether General Equilibrium is even possible, whether its existence is attainable. Walras did provide proofs. However, his proofs were insufficient for the non-linear systems of equations that regularly crop up in supply and demand theory. This was where Lionel McKenzie stepped in. In his 1959 work "On the Existence of General Equilibrium for a Competitive Economy", he utilised Brouwer's fixed point theorem in order to prove the existence of these General Equilibriums.⁽³⁾ His proof, in summary, uses the idea of a "Utility Function" U (which models the individuals' preferences) acting upon a bundle of goods $\{x_1, x_2, \dots, x_n\}$ then by modelling preferences as monotonic (more is better), he demonstrates how consumer preferences are convex, and from that he shows how an equilibrium (or fixed point) has to exist as a result of Brouwer's fixed point theorem.

GAME THEORY

Brouwer's Fixed point theorem also has great use in game theory, especially in the proof of what is referred to as Nash's theorem, named after the father of Game Theory: John Nash. Game theory is concerned with the playing of, and strategies that lead to getting good outcomes from games. A game is defined as a situation whereby multiple 'players' make decisions towards a result which is predicated by the set of circumstances at play. Strategies are hence defined as plans of action that a player will take given the set of circumstances. An optimal strategy doesn't necessarily mean that a player is guaranteed the best outcome every single time but rather that a player would not be able to expect a better outcome of the game by changing their strategy. A Nash's equilibrium is when *all players have a strategy such that even when each player gets to see the other players' strategies, they don't change their strategy.*

For example, suppose that two 'players' are playing a game where they get a decision between two options: option A and option B. If a

player chooses option A, they win £100, if they choose option B, they lose £50. Here the obvious strategy is choosing option A every time, and even if you reveal your strategy to your opponent, they would carry on choosing option A. A Nash equilibrium exists quite obviously for this game. However, game theory is often interested in more interesting games, for example, could an equilibrium be reached if both players lose £100 when they both pick option A?

Remarkably, what John Nash proved was that every n-player game with a finite number of pure strategies has a Nash equilibrium. He accomplished his proof in a similar way that Lionel McKenzie was able to construct a proof for General Equilibriums. To briefly sum it up, by supposing each game to have i players $i \in \{1, \dots, n\}$, each of whom has A_i strategies then each player has a utility function $u_i: A \rightarrow \mathbb{R}$ which considers the sum of each possible set of strategy 's utility multiplied the probability that each combination will be played. The combination of these utility functions must necessarily produce some fixed point by Brouwer's fixed point theorem. Hence, every n-player game with a finite number of pure strategies has a Nash equilibrium.

In our example game, an equilibrium can be reached by both players going for an alternating approach, choosing A and then B whilst the other player chooses B and then A. This results in each player gaining £50 every second go. This is a Nash's equilibrium because even if the two players were to reveal their strategy to their opponent, they would still follow the same strategy. After all, it provides the optimal outcome for both of them.

SOME INTERESTING CONCLUSIONS:

Whilst not being particularly crucial to the modern world, there are some perhaps trivial results of Brouwer's fixed point theorem which are particularly interesting. Here are five such cases.

A CUP OF TEA

If you mix a cup of tea with a spoon, you are in effect, applying a continuous function to a convex object in 3D Euclidean Space. Hence, no matter how much you try, some part of that tea will always end up in the same place that it started in. (This is of course if we remove the discrepancies caused by tea ultimately being made up of particles rather than an infinite number of points, but this fact is still approximately true.)

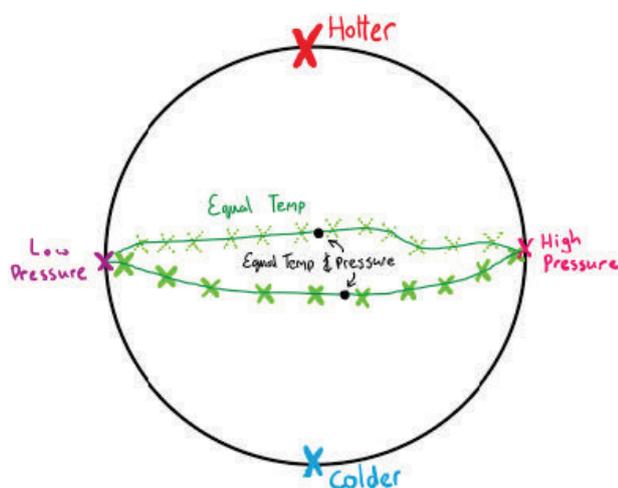
TWO DJS

Suppose you have two DJs. The first one plays a song exactly as it was brought out, with no altering. The second one warps the song, speeding it up in places perhaps to alter the pitch and slowing it down at other times. As long as the first DJ starts before and finishes after the second DJ, it is necessarily true that at least one point in the song, the two DJs will be playing exactly the same part of the song. We can imagine the second DJ as having done a continuous function to a one-dimensional object by warping the song. Hence, Brouwer's fixed point theorem applies.



METEOROLOGY

At any given time, there are at least two points on the Earth where the temperature and atmospheric pressure at those points are entirely identical. A good way of imagining this is to picture two points on the Earth's surface with different temperatures. As one moves from the hotter temperature to the colder temperature, as temperature is gradient, at one point, the temperature must be exactly equal to the average of the two temperatures. Now, one can make this journey in several straight lines around the planet and connect the points where the temperature is the same. Now, we can pick two points on this line that has been created, suppose that they have different pressures, starting at the higher pressure, we can move to the lower pressure and at one point the pressure, as pressure is gradient, must be exactly the average of these two pressures. You can also walk around this line the other way to find another point. Hence, these two points have the same temperature and pressure.



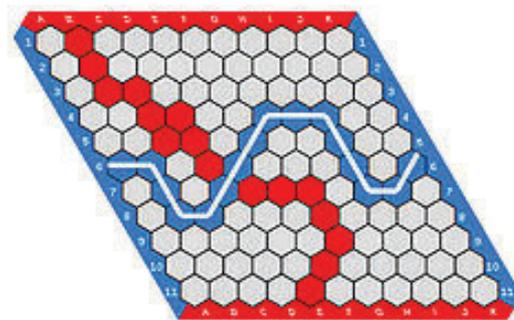
CARTOGRAPHY

If you take a map of any place in the world, say Wales, and make a copy of it. Then you apply a continuous function to the map, enlarge it, rotate it or, even crumple it if you want to. Then we know for a fact that if we take that map and put it on top of the other map, one location on that map will rest on top of the same location on the other. What's more, if we take that map to Wales itself, some point of that map will lie exactly on top of where that point actually is in Wales.

THE GAME OF HEX

If you've ever watched an episode of Blockbusters, you'll be familiar with this game. It was invented by a Danish engineer in 1942 and thoroughly investigated in Princeton by John Nash in 1948. The game involves two players. One plays vertically and the other plays horizontally. The vertical player needs to make a chain of connected hexagons that connects the top to the bottom. The horizontal player needs to do the same from one side to the other. The two players alternate turns. In the example below, the horizontal player is using blue tokens and has won by making a complete chain.

John Nash demonstrated that it is impossible for a game of hex to result in a draw. This can be thought of simply because the only way to fully



block your opponent is to complete your own chain, which would result in your own victory. This is known as in combinatorics as the *Hex Theorem*.

In 2008, David Gale, American mathematics and economics professor at the University of California, Berkeley, used this 'Hex theorem' to produce a combinatorial proof for Brouwer's fixed point theorem.^[4] As Francis Su, a Harvey Mudd College mathematician puts it "Hex implies Brouwer's!"

A BRIEF FINAL THOUGHT

I think that ultimately, I partially disagree with Brouwer's pessimistic neo-intuitionist way of looking at Mathematics. I think that what my IIA shows is how even the most seemingly abstract fields of mathematics (as algebraic topology is often considered to be) seem to be applicable to a spectrum of situations. For this theorem, in particular, it is able to relate not only to the physical world but also to economics and game theory. And further to this, despite its utility, the proofs that underpin the mathematics can still be quite beautiful.



Supramolecular Cages: Their design, chemistry and applications

Salvatore Nigrelli

AN INTRODUCTION TO SUPRAMOLECULAR AND HOST-GUEST CHEMISTRY

Supramolecular chemistry is a notoriously difficult discipline to define because it spans such a broad area of chemistry. Elements of organic, inorganic and physical chemistry – the three fundamental chemistry disciplines – are all deeply involved in the many facets that make up supramolecular chemistry. Some, such as Atwood, choose to define it as ‘The chemistry of the non-covalent bond’. This is because this idea of non-covalent attractions is fundamental to supramolecular chemistry because they are the key building blocks by which supramolecular assemblies can be synthesised. Others, such as Lehn, prefer the definition ‘The chemistry of molecular assemblies and the intermolecular bond’ because supramolecular chemistry aims to utilise these intermolecular forces of attraction to create a larger, functioning molecular assembly.

However, in relation to the supramolecular assemblies that will be discussed throughout my investigation, the definition that I think is most applicable incorporates elements of both of the above definitions: ‘The field of chemistry that deals with the non-covalent interactions between molecules and how these can be utilised to yield functional assemblies with specific physical and chemical properties’.

To properly understand supramolecular chemistry, and the ideas that it presents, it is critical that we understand the history behind it, and the motivations that led to its development.

The first stage in the development of supramolecular chemistry was the creation of the idea of non-covalent interactions. The first non-covalent interactions to be proposed were intermolecular forces of attraction. These were first presented in the French mathematician and geophysicist Alexis Clairaut’s 1736 treatise *‘Theorie de la Figure de la Terre’* (Theory of the Shape of the Earth). Whilst it may seem surprising that intermolecular forces would be presented in a book on three dimensional elliptical geometry, in this seminal work, Clairaut fleetingly proposes the idea that there are tiny attractive forces between small particles that affect their motion. Almost by accident, one of the most fundamental ideas of modern chemistry had been born.

Clairaut’s ground-breaking idea had been largely forgotten for almost a century until the introduction of atomic theory by John Dalton in the early 19th century. As soon as scientists began to postulate the existence of atoms, many also proposed that there could be interactions between atoms of separate molecules. In fact, the thermodynamic implications of such intermolecular attractions were studied in depth by such high profile scientists as Laplace, Maxwell and Boltzmann.

However, a viable mechanism as to how these attractive forces might come about was still lacking until 1873. It was then that the Dutch physicist Johannes Diderik Van Der Waals proposed that the distortion

of electrons around atoms caused by a molecule’s structure would create temporary irregularities in the electric field around molecules (instantaneous dipoles). Such instantaneous dipoles would be able to induce complementary irregularities in separate molecules and thereby cause a small electrostatic attraction between the two molecules. Now that a mechanism had been proposed, scientists from across the world rushed to try and detect these so called Van Der Waals forces, and over the following 40 years a plethora of different intermolecular forces of attraction were discovered, the strongest of which by far was the hydrogen bond discovered in 1912 by Moore and Winmill.

The 1940s and 50s produced another leap in the journey towards supramolecular chemistry. Chemists began to postulate whether it would be possible to use non-covalent interactions like intermolecular forces to manipulate molecular assemblies to create a specific molecular architecture. This seemed unattainable for many years until 1961, when Pedersen synthesised the first crown ether (dibenzo-18-crown-6) and showed that it was able to encapsulate a potassium cation purely using ion-dipole forces - a type of non-covalent interaction (Figure 1).

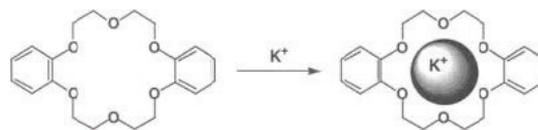


Figure 1 A diagram of K^+ encapsulation by dibenzo-18-crown-6 (Inouye, 2000)

This incredible discovery showed proof of the new possibilities that utilising non-covalent interactions allowed, and thus a new field of chemistry had been born.

Ever since then, the supramolecular structures that have been synthesised have become ever more complex, from cavitands and cages to molecular baskets and tennis balls. In fact, in 1987 the Nobel Prize in Chemistry was awarded to Pedersen, Cram and Lehn for their discovery of the application of non-covalent interactions to make complex molecular assemblies. This shows the vast importance of supramolecular chemistry as a modern chemistry discipline.

As supramolecular chemistry developed further, this idea of a supramolecular chemist’s toolbox began to form. There are four main forms of non-covalent interaction that constitute the ‘tools’ that supramolecular chemists can use to create a functional assembly.

1. ELECTROSTATIC ATTRACTIONS

This encompasses three different types of interaction: ion-ion, ion-dipole and dipole-dipole. All three of these rely on the same fundamental principle that opposite charges experience an attractive force. The charges can be either in the form of fully charged ions, or as dipoles, which are partial charges formed due to uneven electron distribution in a polar covalent bond. This unevenness in polar covalent bonds is

caused by differences in electronegativity of the two bonding atoms, which leads to a larger coefficient of the bonding molecular orbital lying on the more electronegative atom and a larger coefficient of the empty antibonding orbital lying on the more electropositive atom.

Ion-ion interactions are non-directional, since the charge is equally distributed around the charge-carrying species. Ion-dipole or dipole-dipole interactions, however, are directional - since the dipole is on a specific end of the molecule, a particular arrangement must be obtained to maximise the attraction of the interaction (Figure 2).

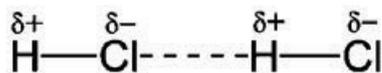


Figure 2 Dipole-dipole interaction between HCl molecules adopting a specific linear arrangement (Lumen, 2020)

Electrostatic interactions are, in general, relatively high in energy, since the large charges involved result in a larger electrostatic force between the molecules compared with most of the other interactions'. In particular, ion-ion interactions have an exceptionally high energy of 250 kJmol^{-1} , which is higher than the energy of even a weak covalent bond – and over 10 times higher than the next strongest non-covalent interaction (hydrogen bonds). But unfortunately, it is rare to find circumstances where ion-ion interactions can be used in supramolecular assemblies, and so ion-dipole and dipole-dipole interactions have proven to be much more useful to supramolecular chemists.

2. DISPERSION FORCES

These weak electrostatic forces are the result of attractions between instantaneous dipoles caused by momentary irregularities in the electron distribution around molecules. They are the only non-covalent interaction that affects every molecule – as long as a molecule has electrons, it will experience dispersion forces. They constitute an extremely delocalised interaction due to their random nature, which makes it very difficult to create supramolecular assemblies that rely on them for encapsulation. One of their few uses to date has been to encapsulate individual atoms that cannot undergo any of the other non-covalent interactions, such as xenon atoms (Figure 3).

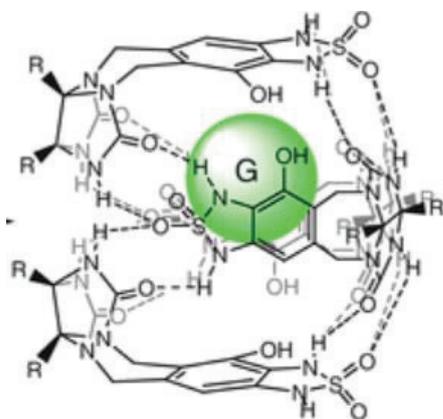


Figure 3 Xenon atom encapsulated in a tennis ball capsule using dispersion forces (Voloshin, Belaya, & Krämer, 2016)

3. π - π STACKING INTERACTIONS

This is the attractive force experienced between two aromatic rings. The exact mechanism behind this interaction is still unknown, but, the most recent theories suggest that it is electrostatic in nature. π - π stacking interactions can adopt only two arrangements – face-to-face and edge-to-face (Figures 4 and 5).

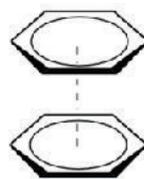


Figure 4 Face-to-face π - π stacking interaction (Rica, 2011)



Figure 5 Edge-to-face π - π stacking interaction (Rica, 2011)

This highly specific geometry makes this interaction extremely useful for supramolecular chemists as it allows for easy synthesis of unusual molecular architectures. In fact, it is believed that the unconventional herringbone crystal structure of benzene is formed to maximise the number of edge-to-face π - π stacking interactions.

4. HYDROGEN BONDS

Only three elements are electronegative enough to take part in hydrogen bonding – fluorine, oxygen and nitrogen. Due to their very high electronegativities, when these elements are bonded to hydrogen, they create a large positive dipole on the hydrogen atom. This positive dipole can then be attracted to the large negative dipole on the electronegative element of another molecule and the result is a large electrostatic interaction. Moreover, since hydrogen bonds form by the lone pair of the electronegative element adding a lone pair of electrons into the antibonding molecular orbital of the other molecule, the position of the antibonding orbital in line with the covalent bond means that hydrogen bonds form a specific molecular geometry and so are highly directional – in fact only very small deviations in the hydrogen bond angle of up to 15° are possible (Chaplin, 2020).

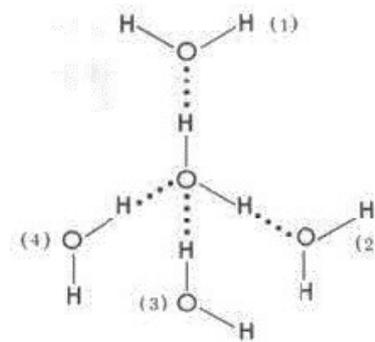


Figure 6 Hydrogen bonding in water (Kimball, 2011)

Both their strength and directionality make hydrogen bonds incredibly useful for supramolecular chemists. Their strength means that very few hydrogen bonds need to be formed to result in the enthalpy change needed to spontaneously encapsulate the desired molecule, and their directionality allows for the formation of molecular assemblies with very specific architectures.

As well as varying hugely in directionality, the non-covalent interactions mentioned above also vary enormously in energy; whereas the average hydrogen bond might have an energy of 20 kJmol^{-1} (Beer, Gale, & Smith, 1999), dispersion forces have a maximum energy of only 2 kJmol^{-1} (Beer, Gale, & Smith, 1999). But to a supramolecular chemist, the differences in energy between interactions is not as important as it may originally seem. What matters more is the number of interactions that can be made, dictated by the architecture of the assembly. For example, although the encapsulation of durene (1,2,4,5-tetramethylbenzene) by a cyclophane relies almost solely on π - π stacking interactions (which have about half of the energy of a hydrogen bond). Due to the geometry of the cyclophane, four such π - π stacking interactions can form, the result of which is quite a strong interaction (with the equivalent energy of two hydrogen bonds) and so the durene molecule is readily encapsulated (Figure 7).

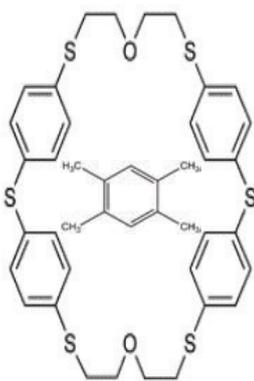


Figure 7 Encapsulation of durene by a cyclophane (Habata, 2008)

These four different types of interactions can be used by supramolecular chemists to create supramolecular assemblies, such as Figure 7, in which a smaller molecule is encapsulated by a larger molecule. This is an idea that will become incredibly important when we begin to think about cage structures later on. There is one principle, above all, that is fundamental when looking at encapsulation and how it works – host-guest chemistry.

In its most basic form, host-guest chemistry is very simple. A smaller molecule (the guest) binds to a larger molecule (the host) via a non-covalent interaction to form a host-guest complex (or supermolecule). To use the example from Figure 7, in this case, the cyclophane is the host, the durene is the guest and the encapsulated durene is the host-guest complex. The nature of the guest can vary hugely depending on the host involved. It can be organic or inorganic, and can vary in size from a large antibiotic to a single atom. For example, in a valinomycin- K^+ complex (Figure 8), the guest is a single K^+ ion.

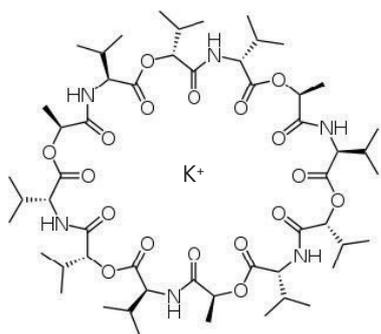


Figure 8 Valinomycin- K^+ complex (Calvero, 2007)

In order for a stable host-guest complex to form, the host and the guest must have complementary electronic character. For example, if the guest has the ability to form hydrogen bonds, then the host should have the ability to form hydrogen bonds with the guest and the hydrogen bonding sites in the host should be arranged to maximise the number of hydrogen bonds that are able to form with the guest. This complementarity in electronic character maximises the strength of the interaction between host and guest, meaning that there is a more negative change in enthalpy when the host-guest complex forms. Having a more negative change in enthalpy means that the host-guest complex is more likely to form because (since $\Delta G = \Delta H - T\Delta S_{\text{sys}}$) it means that the change in Gibbs Free Energy for the host-guest reaction is more likely to be negative, meaning that the reaction is able to happen spontaneously.

But the change in Gibbs Free Energy is often not a good means of calculating the likelihood of a host-guest complex forming, as it is often hard to quantify the change in entropy (ΔS_{sys}) for such a reaction. Instead, a stability constant (also known as a binding constant) for the reaction is calculated. The idea of a stability constant has its roots in organometallic chemistry, where it is used to work out the likelihood of ligand exchange reactions. For host-guest complex formation reactions, it is worked out as followed:

The equation for the reaction can be written in the following way (where H is the host, G is the guest and HG is the host-guest complex):



Since this is a reversible reaction, we can work its equilibrium constant. This is given the symbol K_1 :

$$K_1 = \frac{[\text{HG}]}{[\text{H}][\text{G}]}$$

But there is also a possibility that another guest will be encapsulated in the same host:



The equilibrium constant for this reaction (K_2) is:

$$K_2 = \frac{[\text{HG}_2]}{[\text{HG}][\text{G}]}$$

We can then continue this up to K_n :

$$K_n = \frac{[\text{HG}_n]}{[\text{HG}_{n-1}][\text{G}]}$$

The stability constant (β_n) for any one of these reactions is defined as:

$$\beta_2 = \frac{[\text{HG}_2]}{[\text{H}][\text{G}]^2}$$

Now, we can also see that, if we multiply K_1 and K_2 together, the $[\text{HG}]$ terms cancel, and we are left with β_2 .

Therefore, continuing this process up to K_n it is clear that:

$$\beta_2 = \prod_1^n K_n$$

$$\therefore \beta_2 = \prod_1^n \frac{[\text{HG}_n]}{[\text{HG}_{n-1}][\text{G}]}$$

And so, the total stability constant for a host guest reaction is:

$$\beta_{tot} = \sum_1^n \prod_1^n \frac{[HG_n]}{[HG_{n-1}][G]}$$

This total stability constant provides a measure for how likely it is that at least one host will be encapsulated – a higher stability constant means the reaction has a more negative change in Gibbs Free Energy and so is more likely to happen. Although, for most host-guest complexes, the probability of more than one guest being complexed is very small (a notable exception is provided in Section 9), so $n=1$ provides a reasonable approximation for β_{tot} :

$$\therefore \beta_{tot} \approx \frac{[HG]}{[H][G]}$$

The value for the stability constant depends on a large number of factors, such as the architecture of the host, the type of non-covalent interactions involved, and the relative sizes of the host and guest (which affect the distance over which the non-covalent interactions act). Furthermore, in the next section, we will see that the ease of formation of host-guest complexes involving supramolecular cages as the host also depends heavily on the ease of access of the guest to the inner phase of the cage and the encapsulation mechanism involved.

The journey towards supramolecular chemistry was certainly not a simple one. From the first proposition of intermolecular forces in 1736, it was over 200 years before such interactions were successfully manipulated to create the first host-guest complex. As the field has progressed, a whole plethora of tools and techniques have become available to the supramolecular chemist, such as maximising the number of interactions or using dispersion forces to encapsulate atoms of noble gases. However, it is only by using techniques derived from a variety of different chemistry disciplines, such as stability constants from organometallic chemistry, that supramolecular chemistry was able to develop into the important, revolutionary field that it is today.

SECTION 2: THE MANY TYPES OF SUPRAMOLECULAR CAGES

Supramolecular cage is the term given to a whole zoo of different supramolecular structures, such as carcerands and fullerenes. Each have different structures and binding sites, however, they all have one thing in common – they are all able to form a host-guest complex in which the cage structure completely surrounds the guest, which can vary from a monoatomic cation, in the case of cryptands, to large organic molecules, in the case of hemicarcerands. However, before we look at the applications of these supramolecular cages, it is paramount that we have an idea of what makes each type unique and what makes them a useful means of encapsulation.

Fullerenes are by far the most ubiquitous form of supramolecular cage, of which buckminsterfullerene (or 'Bucky Ball'), discovered in 1985 by Sir Harry Kroto and Robert Curl, is by far the most well-known (Figure 9) – even appearing on most GCSE Chemistry courses. These constitute the simplest supramolecular cages that will be mentioned – they consist of solely carbon atoms arranged in a spherical or ellipsoidal arrangement.

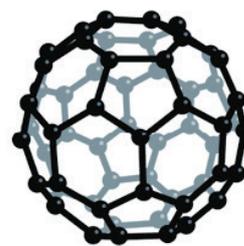


Figure 9 The structure of Buckminsterfullerene (Berne & Mulas, 2015)

These cages are made especially stable by the delocalisation of electrons that can occur. Each carbon atom in the cage only forms three bonds, meaning that there is an extra network of π electrons that can be delocalised – much like in benzene. Moreover, since this effect is experienced in all of the rings that make up the cage, these π electrons can be delocalised over the whole structure of the cage, vastly increasing its stability.

What is not covered when fullerenes are looked at on GCSE or even A Level courses is that they can be used to encapsulate small neutral molecules. The delocalised electrons magnify the dispersion forces within the inner phase of the cage and so can provide a relatively large enthalpy of encapsulation for neutral molecules, making the encapsulation process very energetically favourable. However, by far the most difficult part is getting the small molecules inside the cage so that they can be encapsulated.

The first way that this can be done is to synthesise the fullerene in the presence of the desired guest and hope that some become encapsulated. This, however, gives a relatively low yield because, although the dispersion forces are magnified in fullerenes, they are still weak non-covalent interactions and so they are not strong enough allow the templating effect to occur (where the guest helps to assemble the cage to increase yield of encapsulation – see Section 4) and so the encapsulation is purely based on probability.

The alternative is to construct the cage as normal, and then open a part of it up to allow the guest to become encapsulated, then close the cage again once encapsulation has occurred. This is usually a much more effective way of encapsulating because you can leave the opened host and guest for a long time to maximise encapsulation, whereas in the previous method encapsulation could only occur in the short time taken for the fullerene to assemble. 3,6-diphenylpyridazine is the most common reagent used to open up the fullerene in a so called 'molecular surgery' reaction. When the resulting opened fullerene is treated with oxygen and UV light, followed by 1-hydroxy-N,N-dimethyl-pyridin-4-amine, a large enough opening is formed to allow small molecules such as H_2O to pass into the cage and become encapsulated (Figure 10).

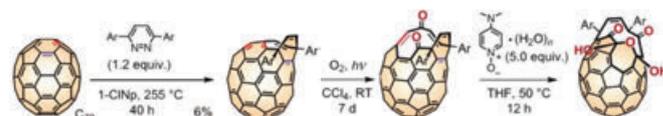


Figure 10 The 'molecular surgery' reaction to open up the fullerene (Gakh, 2018)

Once the guest has been encapsulated, the opening is closed up by first reacting the open cage with triisopropylphosphine, and then 1-phenyl-2,5-pyrrolidinedione (also known as succinimide) to return the cage back to its fullerene structure (Figure 11).

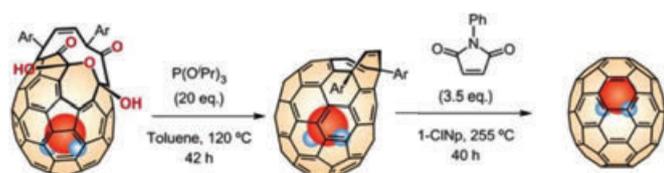


Figure 11 The reaction that closes the fullerene after encapsulation (Gakh, 2018)

However, the yield for the first stage of the molecular surgery reaction is only 6%, which hugely limits any potential applications of fullerene-based host-guest complexes, and furthermore, fullerenes such as buckminsterfullerene, on the molecular scale, are not that large and so the largest guest that has been encapsulated in a fullerene to date is only CH₄ (the simplest and smallest organic molecule). This puts further limitations on the utility of such fullerene cages. If encapsulation of larger molecules with higher yields is needed, we have to look past fullerenes and towards more complex cage structures – carcerands are one such example.

Carcerands, whose name derives from the Latin *carcer* meaning prison, were among the first supramolecular cages to be synthesised in the late 1960s by Donald Cram. They consist of two bowl shaped molecules, called cavitands, (Figure 12) linked by a number of spacer groups.

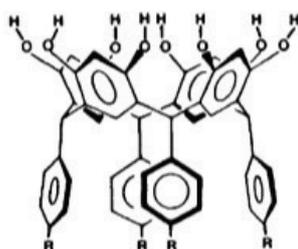


Figure 12 The structure of a cavitand synthesised by Cram in the late 1960s (Cram & Cram, 1994)

Carcerands, unlike fullerenes, have the incredibly useful property that, by changing the length of the spacer groups used, the size of the inner phase can easily be changed so that the optimum inner-phase size for the guest molecule can be achieved (Figure 13).

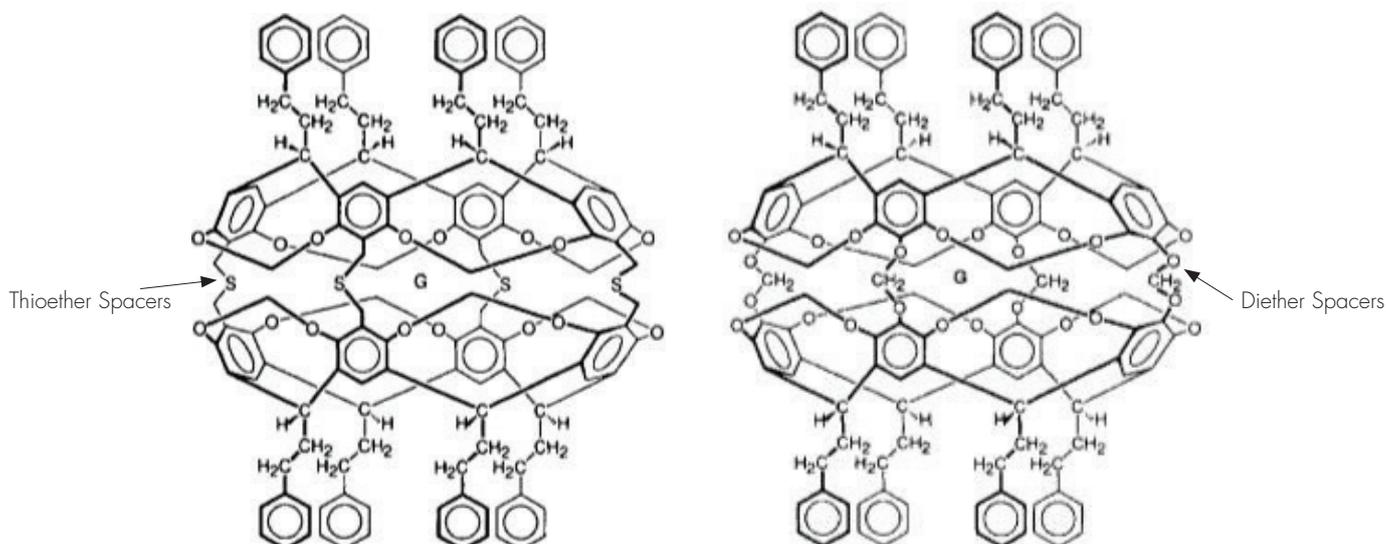


Figure 13 Two carcerands synthesised by Cram with different spacer groups and so different inner phase sizes. The left one has thioether spacer groups, the right one has diether ones. (Cram & Cram, 1994)

While researching carcerands at the University of Parma in the late 1990s, the Italian supramolecular chemist Enrico Dalcanale noted that, in the presence of transition metal atoms in the spacer groups, the percentage yield for the synthesis of carcerands was 87% - making it by far the most efficient synthesis of any supramolecular cage (Figure 14). This was particularly striking considering that the assembly of carcerands is usually an entropically unfavourable process. This remarkable result has subsequently been attributed to two factors. The first is that the interaction between the transition metal atoms in the spacer groups and the guest help to 'template' the assembly and bring the two cavitands close enough to bond to each other via spacer groups. The second is that, once one spacer group forms between the two cavitands, the remaining spacer groups are now very close to their intended bonding sites and so the remaining bonds form extremely quickly as the reaction has become an intramolecular one – it no longer needs to wait for a collision to happen.

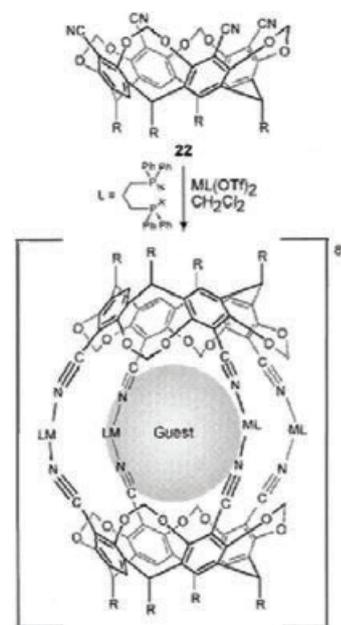


Figure 14 A generalised form of the Dalcanale's templated synthesis of carcerands. In Dalcanale's original research, M is Palladium and the guest is C₁₁H₂₄. (Steinke & Vilar, 2019)

Therefore, if, as the Dalcanele synthesis suggests, the guest can be involved in the synthesis of carcerands, unlike fullerenes, a separate reaction to insert the guest is not required, making the encapsulation process much more efficient. Furthermore, guests that can form stronger non-covalent interactions with the cavitands such as ions (which can undergo strong electrostatic interactions) or larger guests (which cause much stronger dispersion forces) make the process of drawing the cavitands together to bond have a much more negative change in enthalpy, causing a more negative change in Gibbs Free Energy and so a larger stability constant and larger yield of host-guest complexes. This means that carcerands are perfectly suited to encapsulate large guests. For example, the yield for the encapsulation of N,N-dimethylethylamide (a relatively large guest molecule in host-guest chemistry) is 57% (Cram & Cram, 1994), whereas the yield for the encapsulation of neutral argon atoms in the same carcerand is only 0.67% (Cram & Cram, 1994).

It was noticed by Cram in his initial studies on the first carcerands that there was only ever one guest in a carcerand at a time, no matter how large the inner phase was. He attributed this unusual result to the billiard ball effect. As the two guest molecules move around the inner phase of the carcerand, they collide. During the collision, the guest that is less strongly attracted to the cage will be given a larger amount of kinetic energy than the other guest. As more such collisions occur, eventually one of the guests will gain enough kinetic energy to overcome the electron-electron repulsion between the guest and the cage walls and escape the cage, leaving only one guest molecule in the carcerand. What made the situation even more unusual is that, once there was only one guest in the carcerand, it proved extremely difficult to remove the guest. Even if you increased the temperature, and so gave the guest a large amount of kinetic energy, the repulsion between the guest and the cage walls proved to be too strong and so the guest remained in the cage until a high enough temperature was reached that the cage itself decomposed.

However, if the spacer groups were very large, it was a completely different story. At temperatures only slightly higher than room temperature, the repulsion effects were weak enough, because of the increased distance that they acted over, and the guest had enough kinetic energy, to completely escape the cage. This effect was discovered using $^1\text{H-NMR}$ of such cages with organic guests. For example, when Warmuth heated a carcerand containing benzyne, the following $^1\text{H-NMR}$ spectra were obtained (Figure 15).

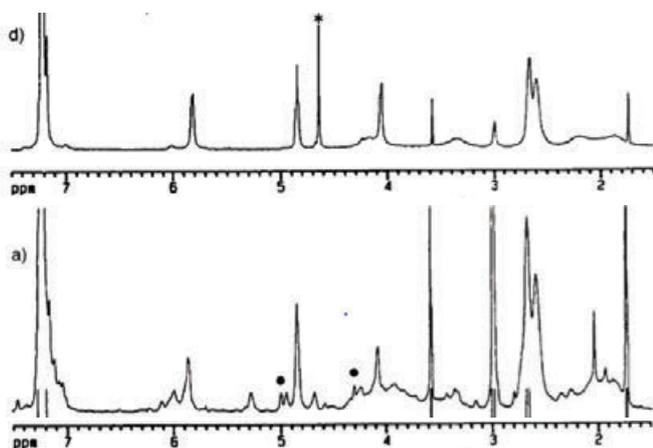


Figure 15 The $^1\text{H-NMR}$ spectra obtained by Warmuth before heating (top) and after heating (bottom) (Warmuth, 1997)

These spectra clearly show that, after heating, the peak at 4.6 ppm (marked with an asterisk), which corresponds to the benzyne hydrogens disappears – the other inconsistencies were determined to be due to different solvent interactions. This disappearing peak therefore shows that, during heating, the guest can completely escape the carcerand and return to the solution. Such carcerands that have this remarkable ability to allow the guest to escape during heating are referred to as hemicarcerands (Figure 16).

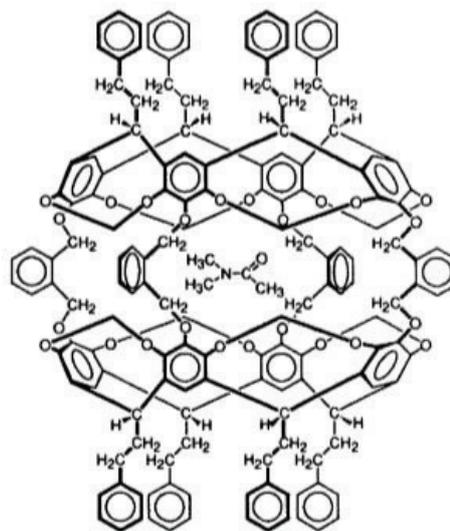


Figure 16 One of the first hemicarcerands synthesised by Cram with benzyl diether spacer groups (Cram & Cram, 1994)

However, it is extremely difficult to control the kinetic energy of individual molecules; at any given temperature, the kinetic energy of molecules in a sample will vary according to the Maxwell-Boltzmann distribution. Therefore, the half-temperature, which is the temperature at which half of the cages have released their guest, is usually more useful to supramolecular chemists. This is determined by performing NMR titrations of the hemicarcerands at a variety of different temperatures to determine the concentration of decapsulated guest molecules.

The temperature at which escape can occur depends on a variety of factors such as the size of the inner phase (which affects the strength of the non-covalent interactions that the guest experiences) and the distance between the spacer groups (which affects the strength of the repulsion between the cage structure and the guest). For example, it was found that if slanted spacer groups were used, i.e. spacer groups that are not connected to their perpendicular bonding site, the size of the gaps in the cage structure increases so the half temperature is lower – the hemicarcerand in Figure 17 has a half temperature of just 53°C (Cram & Cram, 1994), whereas it is 70°C (Cram & Cram, 1994) for the hemicarcerand in Figure 16.

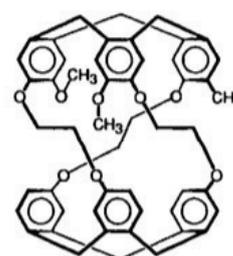


Figure 17 A hemicarcerand with slanted ethyl diether spacer groups (Cram & Cram, 1994)

So, hemicarcerands provide a crude thermal release mechanism for supramolecular cages. We will see in Section 5 that more effective photo release mechanisms can be designed – but these usually rely on a different type of supramolecular cage – coordination cages.

As the name suggests, coordination cages are supramolecular cages derived from transition metals and the unique coordination geometry that they allow. Transition metals have already proven to be useful in the Dalcanale synthesis of carcerands, however, in coordination cages, the difference is that the cage structure is built around the transition metals, allowing for very specific geometries to develop (a more detailed look at transition metal geometries is provided in Section 3). In particular, two geometries are particularly useful in the synthesis of useful coordination cages – pseudo-octahedral and square planar.

The pseudo octahedral geometry around d^6 transition metal atoms such as cobalt (III) have the incredibly useful ability of providing ligand binding sites in a tetrahedral arrangement, and so, if bidentate bridging ligands are used to connect four cobalt (III) atoms, a tetrahedral coordination cage is formed with its edges made from the chosen ligands (Figure 18). This means that the size of the inner phase can easily be altered by changing the length of the bidentate ligands used, meaning that even very large guests can be encapsulated. These tetrahedral cages are particularly useful to supramolecular chemists due to their incredibly high T_d symmetry and so have a whole host of different applications, such as controlling the reactivity of alkyl ammonium guests (Zhang & Yang, 2018).

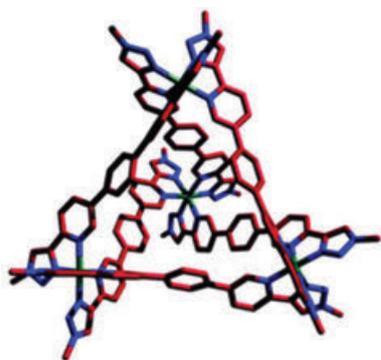


Figure 18 A 3D representation of a tetrahedral coordination cage made using cobalt (III) atoms (Symmers & Burke, 2015)

One other property of cobalt (III) coordination cages makes them particularly attractive to supramolecular chemists. As d^6 complexes, such as those based on cobalt (III), have a high crystal field splitting energy, they have a higher stabilisation of the low energy T_{2g} molecular orbital and a high destabilisation of the e_g high energy molecular orbital (Figure 19). This stabilisation/destabilisation process makes the cobalt (III) complexes inhabit a low energy state and so they are extraordinarily stable – the stability constant for cobalt (III) complexes is 10^{30} times larger than that of cobalt (II) complexes (Housecroft & Sharpe, 2001), which have a low crystal field splitting energy. Therefore, coordination cages based on cobalt (III) atoms are also exceptionally stable, further improving their potential applications.

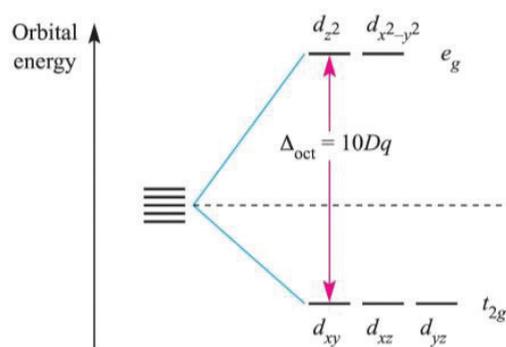


Figure 19 An energy level diagram illustrating the crystal field splitting energy in $Co(III)$ complexes (Lufaso, 2020)

The other geometry that is often used to make coordination cages is the square planar geometry commonly seen in complexes of d^8 elements such as palladium and platinum due to their unusual dsp^2 hybridisation. If bidentate bridging ligands are used to link two or more d^8 metal cations such as palladium (II), a desirable multifaced coordination cage is formed (Figure 20). The size of the inner phase can easily be controlled by changing the length or the bond angles in the bidentate ligands used.

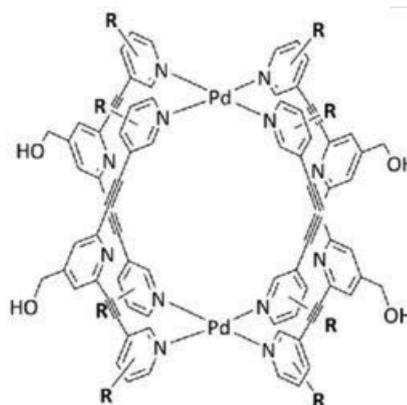


Figure 20 A coordination cage based on $Pd Pd^{2+}$ ions and tripolyridyl bidentate ligands (Crowley, Preston, & Lewis, 2016)

By changing the chemical properties of the ligands, it is also possible to design such coordination cages for specific purposes, for example, if aptamers (short, single stranded DNA or RNA molecules) are used to bridge the palladium centres (Figure 21), the cage's affinity for titanium surfaces vastly increases (Ikemi, et al., 2010) and so the cages can be used to greatly enhance their guest's capability to take part in titanium catalysed reactions.

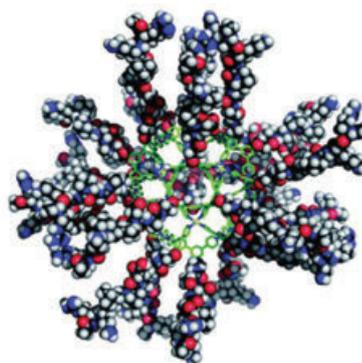
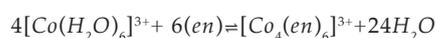


Figure 21 An icosahedral Pd^{2+} based coordination cage with aptamer bridging ligands (Ikemi, et al., 2010)

Curiously, the fact that the ligands bridge two transition metal atoms in both geometries hugely increases the stability of the cage through something called the chelate effect (the same effect occurs if a bidentate ligand bonds twice to the same metal atom). This stability arises from the entropic favourability of the ligand substitution reactions required to form the cage. For example, consider the reaction through which bidentate ligands (such as en – a common shorthand used for ethylenediamine) react with $[\text{Co}(\text{H}_2\text{O})_6]^{3+}$ complexes to form the tetrahedral cage in Figure 18:



On the left hand side, there are 10 species, whereas on the right hand side there are 25, including 24 high entropy liquid water species. Therefore, the right hand side is much more disordered, so there is a large positive change in entropy of the system for this reaction, and so the reaction has a large negative change in Gibbs Free Energy, meaning that the tetrahedral cage formed has a very high stability constant and so is very stable.

Therefore, the chelate effect helps to make such coordination cages exceptionally stable.

The last major type of supramolecular cages are cryptands, named from the Greek κρυπτείν, meaning 'to hide' for their ability to encapsulate small cations, these cages are commonly described as three dimensional crown ethers (see Section 1) and were first synthesised in 1968 by Dietrich, Lehn and Sauvage, making them, along with carcerands, among the first supramolecular cages to be discovered. They are named using a naming system devised by Lehn according to the number of oxygen atoms in each of the three linking groups. For example, a [2,2,2] cryptand has two such oxygen atoms in each group. (Figure 22).

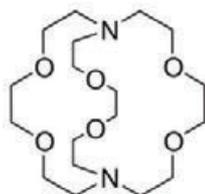


Figure 22 The structure of a [2,2,2] cryptand (Sigma Aldrich, 2020)

In order to be synthesised in any sort of high yield, high dilution techniques must be used to synthesise cryptands. This consists of solutions of each reactant being added dropwise into a large quantity of solvent. This encourages the formation of cryptands rather than poly ether amines because the extremely low concentration of intermediate means that collisions are very infrequent, so the intramolecular cyclisation reaction is favoured, meaning that cyclic cryptands are produced in high yield. Furthermore, cyclisation has a smaller change in entropy than polymerisation, so is less entropically unfavourable than polymerisation in the high disorder environment at low concentrations and so occurs at a much higher rate.

Cryptands have high stability constants - a magnitude of 10^4 higher than crown ethers (Beer, Gale, & Smith, 1999) – when encapsulating monoatomic cations. This high stability constant is due to two main reasons. The first is that, in cryptands, due to the charge symmetry of the cations that they encapsulate, all of the oxygen atoms on the linking groups can form strong ion-dipole interactions. The combination of

all of these strong interactions leads to a large negative enthalpy of encapsulation. The second is a solvent effect when encapsulation occurs in aqueous solvent. The metal cations before encapsulation are strongly solvated by the polar water molecules, but when encapsulation occurs, the interactions between the cation and the water molecules must break, causing the release of a large number of water molecules. This process increases the number of free species in the system, increasing the overall disorder and so causing a large positive change in entropy of the system for the encapsulation process. The combination of these enthalpic and entropic effects leads to a very large decrease in Gibbs Free Energy of encapsulation, giving cryptands a very high stability constant.

Other, more exotic forms of cage structures based on hydrogen bonding also exist, such as the tennis ball capsules and cylindrical sliding cages discovered by the MIT supramolecular chemist Julius Rebek in the late 1990s (Figure 23). However, applications of these so far has been limited to encapsulating neutral guests such as individual xenon atoms, although more important applications such as their potential use as nanoreactors has been proposed. Therefore, the applications of supramolecular cages in Sections 6,7 and 8 will focus on those of the more traditional cage designs such as carcerands and coordination cages.

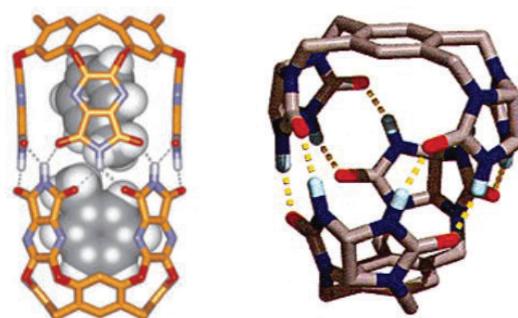


Figure 23 Some of the exotic cages discovered by Rebek: cylindrical sliding cage (Left) and tennis ball capsule (Right) (Steinke & Vilar, 2019)

Supramolecular cages come in a wide variety of different forms, from fullerenes, to hemicarcerands to cryptands. Each different type has its own appeal to supramolecular chemists, whether that be carcerands' ability to encapsulate very large guests, or how coordination cages can exploit the chelate effect and crystal field splitting energies to form exceptionally stable complexes. With the synthesis of ever more exotic cage designs, such as tennis ball capsules and cylindrical sliding cages, one can only begin to imagine the bold, exciting possibilities that the future holds.

SECTION 3: HOW A CAGE CAN BE DESIGNED WITH PARTICULAR PROPERTIES

The potential applications of supramolecular cages rest heavily on the properties of the cage. For example, for cages used in drug delivery (Section 8) water solubility is crucial, or if the cage is required for molecular sensors (Section 7) the geometry of the cage is extremely important. So, the question stands: how can we make sure that the supramolecular cage has the properties that we require? In this section, I will be examining how two important properties of cages – solubility

and geometry – can be manipulated to suit the cage's function.

Solubility can be broadly split into two distinct areas – solubility in water, and solubility in non-polar organic solvents, such as cyclohexane. Although solvents exist that do not fall into either category – propanone is an example of such a solvent – water and organic solvents are by far the most common and important solvents for supramolecular cages.

So, what makes a molecule soluble in water? In pure liquid water, strong hydrogen bonds exist between the water molecules (see Section 1 Figure 6). For something to dissolve in water, some of these hydrogen bonds must be broken and replaced by interactions between the water and the solute. Breaking these hydrogen bonds requires a large amount of energy, so unless a similar amount of energy can be released due to the new interactions between water molecules and the solute (in reality this can be slightly less than the energy of the original hydrogen bonds due to the entropic favourability of dissolving), the dissolving process will be very endothermic, and so the change in Gibbs Free Energy is likely to be positive – meaning that the dissolving process will not happen spontaneously. Molecules that can form substantially strong interactions with water molecules for the dissolving process to occur spontaneously are called hydrophilic. Hydrophilic molecules often have high polarity, usually due to either polar bonds or hydrogen bond acceptors/donors. This polarity allows the solute to form strong interactions with many water molecules called hydration spheres (Figure 24); the sum of the energy released by the formation of all of these small interactions with water molecules in the hydration sphere is more than enough energy to allow the solute to dissolve.

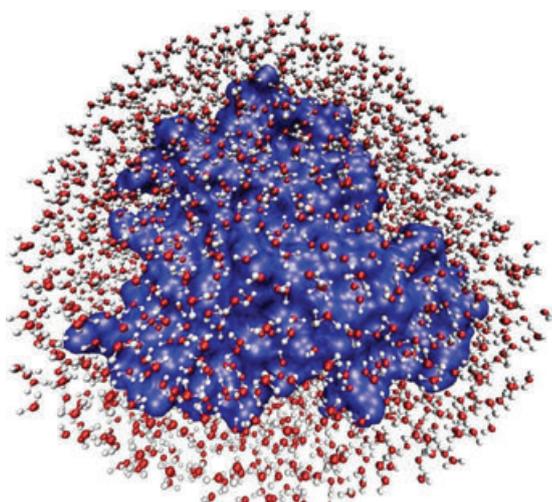


Figure 24 A hydration sphere that has formed around myoglobin - a water soluble protein made from hydrophilic amino acids (Fraunfelder & Chen, 2009)

Therefore, a supramolecular cage can be made more soluble in water by making its structure more hydrophilic. This can be done by making the cage structure itself feature more polar bonds or hydrogen bond acceptors and donors, however it is usually easier to do it by adding hydrophilic side chains to the cage structure. Hydrophilic side chains are groups of atoms that can be attached to the outside of the cage structure which have a high polarity and so increase the solubility of the entire cage. Popular choices for such hydrophilic side chains are polypeptides made from the nine hydrophilic amino acids: serine, threonine, aspartic acid, glutamine, cysteine, asparagine, glutamic acid, arginine and histidine. However, hydrophilic polymer side chains such as polyethylene glycol (PEG) (Figure 25) are also commonly used

because its large chain length allows for a large number of polar bonds and so it is hydrophilic enough to make formerly insoluble cage structures water soluble.

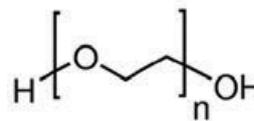


Figure 25 Polyethylene glycol - a hydrophilic polymer commonly used as a hydrophilic side chain in supramolecular cages (Sigma Aldrich, 2013)

The opposite reasons explain why a molecule is soluble in organic solvents. Molecules with high polarity have strong intermolecular forces between each other, so when such molecules are dissolved, these strong interactions must be broken and replaced with stronger interactions between the solvent and the solute. However, for non-polar organic solvents, the only interactions able to form between solute and solvent are dispersion forces which are weak. Therefore, it is very energetically unfavourable for molecules with high polarity to dissolve in non-polar organic solvents. Instead, the molecules best suited to dissolving in non-polar organic solvents are ones where only dispersion forces exist between the solute molecules in their undissolved state (i.e. molecules with low polarity) – so the reformation of dispersion forces with the solvent upon dissolving releases enough energy to make the dissolving process favourable. As a result, the molecules best at dissolving in non-polar organic solvents are usually extremely bad at dissolving in water – and so are called hydrophobic.

In exactly the same way as for hydrophilic cages, hydrophobic side chains can be used to make a cage more soluble in non-polar organic solvents. Such side chains tend to be bulky and contain lots of bonds between elements of similar electronegativities – which give it a low polarity. Common choices include polypeptides of the seven hydrophobic amino acids: glycine, proline, phenylalanine, alanine, isoleucine, leucine and valine. However, in general, cage structures tend to be bulky and have low polarity – since benzene rings and alkyl chains are commonly used to make the cage structure itself, so adding side chains to increase a cage's hydrophobicity is not usually required.

The geometry of a cage is hugely important, if it is to function in the desired manner, for a whole variety of reasons. The geometry of the cage controls the position of the binding sites. For host-guest interactions involving highly directional non-covalent interactions, such as hydrogen bonds this is vital because a deviation of the binding sites from the optimal positions can vastly decrease the strength of the interaction, and so greatly decrease the stability constant for the host-guest complex (an example this can be seen in Section 9). The geometry of a cage can also play a very important role in its stability and ease of assembly. For example, if a coordination cage consists of bridging or multidentate ligands, by the chelate effect (Section 2), the stability constant for the cage will increase and so the assembly of the cage will be a much more energetically favourable process and so it is more likely that successful self-assembly will occur.

Arguably the most important factor to consider when designing a cage with a particular geometry is choosing the right centre. The centre of a cage is simply the atom or group of atoms that a supramolecular cage is built around. For many cages (such as most cryptands) the centre can be as simple as a single nitrogen atom or a benzene ring (Figure 26)

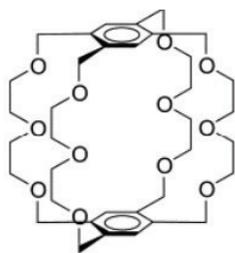


Figure 26 A 3,3,3,3 cryptand which has a benzene ring as its centre (Pettinari, 2003)

However, to obtain more specific and complex geometries, typical p-block element based centres are much less useful. Instead, it is necessary to use coordination chemistry and d-block elements to obtain the desired geometry. Coordination chemistry is simply the chemistry of dative covalent bonds. More specifically, it is the branch of chemistry that deals with ligand-metal interactions and the formation of complexes using ligands and d-block elements.

The coordination chemistry of d-block elements allows for much greater variation in geometry than the valence shell electron pair repulsion (VSEPR) theory that controls the molecular geometry of p-block elements. This is because d-block elements have nine atomic orbitals in their outer shells whereas p-block elements have only four. There are more atomic orbital combinations when making molecular orbitals for d-block elements than p-block, allowing for more variation in geometry. In addition, in coordination chemistry, non-bonding molecular orbitals, the equivalent of lone pairs in VSEPR theory, exert much less of an influence in the overall geometry than lone pairs do for p-block elements. This means that there are fewer constraints on the molecular geometry for elements in the d-block than the p-block.

To understand the sheer variety of geometries made possible by coordination chemistry, we need to use something called a coordination number. A coordination number, a term coined by Swiss chemist Alfred Werner in the 1910s is the secondary valency possessed by transition metal elements. The primary valency is the oxidation state of the metal atom, and the secondary valency (coordination number) is the total number of ligands bonded to the metal atom (bidentate ligands count twice when calculating the coordination number). Much like in VSEPR theory, where the number of bonding and lone pairs determines the geometry, for d-block elements it is the coordination number that determines the geometry.

For low coordination numbers (1-4), the geometries that occur are very similar to those that we would expect from VSEPR theory for example the palladium complex PdH_3 has a trigonal planar geometry and the titanium complex TiCl_4 is tetrahedral (Figure 27).

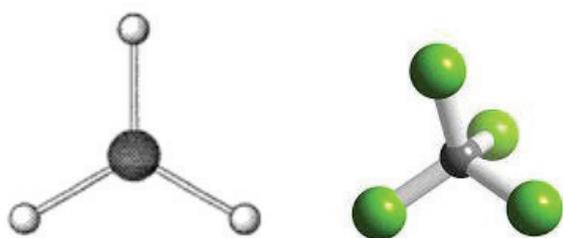


Figure 27 3D representations of PdH_3 (Left) and TiCl_4 (Right) (Olofsson, Kritikos, & Noreus, 1998) (University of Liverpool, 2020)

The one exception is a square planar geometry. Molecules with square planar geometry are quite rare in VSEPR theory and tend to be limited to unusual noble gas compounds such as XeF_4 . However, a square planar geometry is very common amongst d-block elements with a coordination number of 4 – especially d^8 group elements such as palladium and platinum for whom the dsp^2 hybridisation in their molecular orbitals makes a square planar geometry very favourable. A common example is the anticancer drug cis-platin, which features a square planar geometry around the central platinum atom (Figure 28).

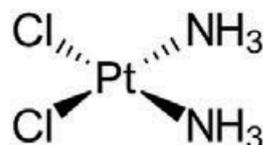


Figure 28 The structure of cis-platin, which contains platinum in a square planar geometry (Benr 2012)

A square planar geometry is extremely useful when designing coordination cages, because it allows for a cage to contain four parallel ligands – something that comes in handy when designing a receptor to ensure strong binding of guests with square planar and octahedral geometries. An example of the importance of such cages is the cage in Figure 29, which exploits the square planar geometry around the two palladium atoms to construct a coordination cage able to encapsulate cis-platin (Figure 28) and vastly improve the effectiveness of its drug delivery mechanism.

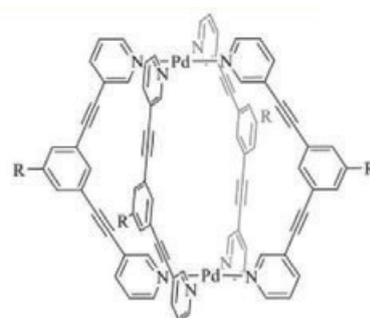


Figure 29 A coordination cage with two square planar palladium centres (Woods, et al., 2019)

As the coordination number of a metal increases, the molecular orbitals that form and the orbital hybridisation that occurs can become much more complicated. This leads to a whole host of wacky geometries such as pentagonal bipyramidal in $[\text{ZrF}_7]^{3-}$ (Figure 30) for a coordination number of 7, and tricapped trigonal prismatic for a coordination number of 9 in complexes such as $[\text{ReH}_9]^{2-}$ (Figure 30)

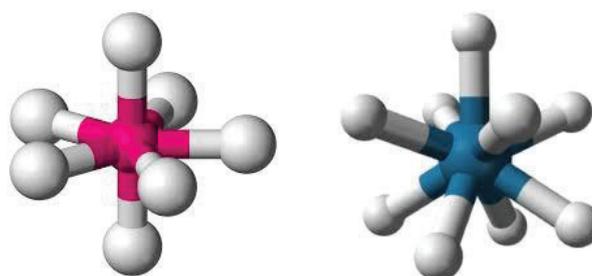


Figure 30 3D representations of $[\text{ZrF}_7]^{3-}$ (Left) and $[\text{ReH}_9]^{2-}$ (Right) (Mills, 2008)

Although some of the weird and wonderful geometries obtained – particularly those with large odd numbered coordination numbers – are simply too irregular to every find use in a supramolecular cage, many unusual geometries have been incredibly useful in creating specific cage designs – for example, the cage designed in Section 9 relies heavily on the unusual trigonal prismatic geometry around two molybdenum atoms (with coordination numbers of 6), and in the cage in Figure 31, which is used to encapsulate benzoic acid derivatives, the multidentate nature of the ligands make an octahedral geometry (allowed by the coordination number of 6 for the zirconium atoms) very energetically favourable.

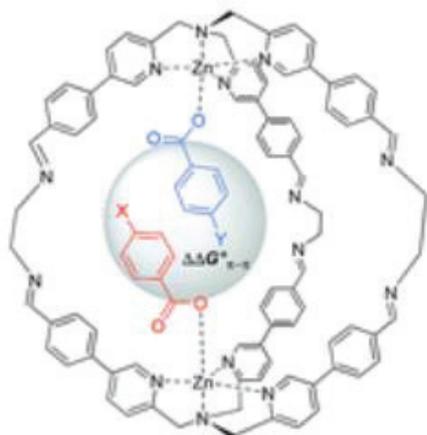


Figure 31 A coordination cage based on two octahedral zirconium centres in a host-guest complex with two benzoic acid derivative guests (Bravin, Guidetti, Licini, & Zonta, 2019)

So clearly, both the solubility and the geometry of supramolecular cages are hugely important in ensuring that it has the desired properties. Simple adaptations to the cage structure, such as adding hydrophilic side chains like PEG, or using d-block metal centres to take full advantage of the unique geometry that they allow, play an integral role in helping to manipulate the properties of the cage so that it is perfectly suited to carry out its function.

SECTION 4: SELF-ASSEMBLY TECHNIQUES

Since it is not possible to individually construct supramolecular complexes, it is the job of the supramolecular chemist to work out how to make sure that the starting molecules come together in the desired arrangement. At the heart of this process is this idea of self-assembly.

In its basics, self-assembly is simply the reversible assembly of a specific host-guest complex. More specifically, is the mechanism by which a disordered system of component molecules forms a structure with high levels of organisation due to the precise small-scale interactions between them. An example of the supramolecular assembly of an icosahedral cage structure from two types of component molecule is shown in Figure 32.

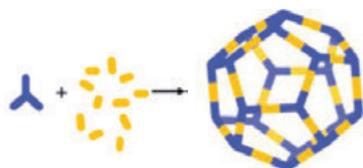


Figure 32 The self-assembly of an icosahedral cage structure from two types of component molecules (Davis, Yeh, & Raymond, 2002)

In most self-assembly schemes, having symmetrical component molecules is essential, otherwise it is very difficult to control the assembly and make sure that the desired host-guest complex forms. Therefore, Platonic solids such as icosahedra, tetrahedra, and octahedra are very useful structures for supramolecular cages (particularly coordination cages) due to their high degrees of symmetry, meaning that they can easily be synthesised from symmetric components.

However, the immediate problem faced by self-assembly is the second law of thermodynamics. Creating an ordered system from a disordered one – as self-assembly aims to do – is very entropically unfavourable and so causes a very negative change in entropy of the system, which would make the change in Gibbs Free Energy for the reaction much less negative and so the stability constant for the host-guest complex would be extremely low. Fortunately, supramolecular chemists have devised a number of ways of increasing the entropy of the self assembly process meaning that the stability constants of the intended host-guest complexes are much higher.

The overall change in entropy (ΔS_{agg}) for a typical self-assembly reactions is given by the following equation (Bergstrom, 2011):

$$\Delta S_{agg} = -k(\ln(\varphi_N) - N\ln(\varphi_{free}))$$

Where N is the total number of component molecules, φ_{free} is the volume ratio of the component molecules, φ_N is the volume ratio of the host-guest complex that forms and k is a positive constant. To minimise the increase in entropy for the self-assembly process, ΔS_{agg} must be as little below zero as possible. So, it is clear that, for this to occur, we want φ_N to be as high as possible and φ_{free} to be as low as possible. This can be achieved by using a saturated solution of the component molecules in a solvent that has a high affinity for the component molecules, but a very low affinity for the self host-guest so that it precipitates out of the solution. By making these changes to the nature of the solution used for the self-assembly, ΔS_{agg} can be minimised so that the stability constant for the host-guest complex is as high as possible.

Another popular way for supramolecular chemists to solve the issue of entropy is to exploit the hydrophobic effect. When supramolecular cages with hydrophobic inner phases are assembled in aqueous solution, as the cage structure begins to form, water molecules arrange themselves in structured arrays inside the inner phase, but do not form interactions with the hydrophobic cage walls (Figure 33).

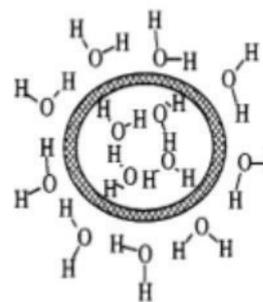


Figure 33 The structured array of water molecules inside a hydrophobic supramolecular cage compared to the disordered arrangement outside (Thomas, 2017)

When the host becomes encapsulated, this water becomes displaced and returns into the aqueous solution. As it does so, the structured array of water molecules breaks down, which is very entropically favourable and the water molecules form more hydrogen bonds, causing a

favourable change in enthalpy. The combination of these entropic and enthalpic effects causes the encapsulation process to have a more negative change in Gibbs Free energy than it otherwise would, and so the host-guest complex that forms has a much higher stability constant.

In some circumstances, however, since the change in Gibbs Free energy is a function of both changes in entropy and enthalpy ($\Delta G = \Delta H - \Delta S_{\text{sys}}$) even if there is a negative change in entropy of the system, if there is a sufficiently negative change in enthalpy, there will still be a negative change in Gibbs Free Energy and so a high stability constant. This is a strategy that is often used when assembling very large supramolecular assemblies. If, during the self-assembly, a large number of high energy covalent bonds can form, the result will be a significantly negative change in enthalpy and so a high stability constant.

In the early years of supramolecular chemistry, organic synthesis provided the strategies for self-assembly. For example, high dilution techniques, which had been known and used by organic chemists many years earlier to synthesise macrocyclic rings, were exploited by Lenh, Diedrich and Sauvage in 1968 in the self-assembly of the first cryptand (Section 2). However, as supramolecular cages became ever more complicated in their structures, it became clear that organic synthesis methods would no longer be useful – in the synthesis of the first carcerands, the three stage process required first the synthesis of octols from resorcinols, then the synthesis of cavitands from octols and then the synthesis of carcerands from cavitands (Figure 34). The multistage nature of this process meant that the final yield was only 51%. There had to be a more effective way to synthesise supramolecular cages.

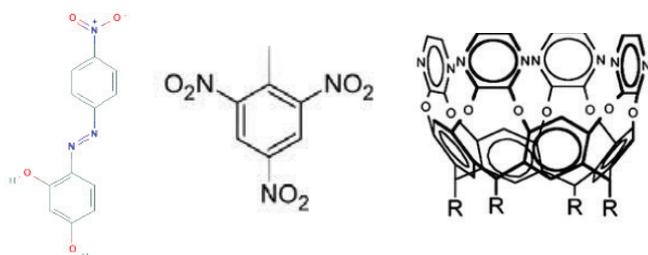


Figure 34 Three organic intermediates in the synthesis of carcerands - from left to right - resorcinols, octols and cavitands (Pub Chem, 2020), (Enacademic, 2020), (Korotcenkov, 2013)

In the end, the solution came from applying a principle from organometallic chemistry known as templating. Templating works on the principle that another molecule or ion can be used to stimulate the assembly of the desired arrangement. In organometallic chemistry templating is used to ensure the correct geometry occurs during ligand substitution reactions. For example, the use of nickel (II) atoms as a templating agent in the dialkylation of a nickel dithiolate locks the conformation of the complex, ensuring the formation of a multidentate ligand based nickel (II) complex, rather than the polymer that would form if the nickel atoms were not present (Figure 35).

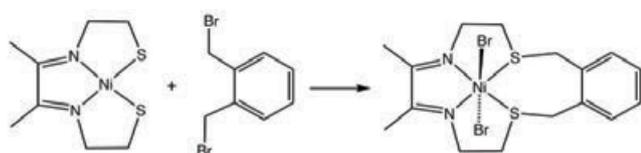


Figure 35 The equation for the nickel templated dialkylation of a nickel dithiolate (Daryle & Thompson, 1964)

With templating in supramolecular chemistry, a field worked on extensively by the prolific Japanese supramolecular chemist Makoto Fujita, a whole variety of different species can be used as a templating agent, including metal atoms, cations, anions, and even simple organic molecules. Templated self assemblies, such as the Dalcanele synthesis of carcerands outlined in Section 2, can have yields as high as 87% (Steinke & Vilar, 2019) – over 36% higher than the yield of carcerands using organic based self-assembly. Moreover, if the templating agent is the desired guest, an extremely high yield of encapsulation is also obtained – since almost all of the hosts that form will already contain the guest inside.

Modern Supramolecular chemistry divides templating self-assembly of supramolecular cages into two distinct areas: edge directed and face directed. Both work on the principle that the non-covalent interactions that form between the templating agent and the component molecules bring the component molecules into close proximity, which allows for easy covalent or coordination bond formation to construct the structure of the cage, but they do so in very different ways.

In edge directed templated self-assembly, the strong non-covalent interactions between the component molecules and the templating agent are used to build up the edges of the cage structure. Hydrogen bonding is commonly used because its high strength means that there is a greater change in enthalpy upon the formation of the interaction between the component molecules and the template, and their directional nature allows for the component molecules to be positioned in the correct arrangement to form the edges of the cage structure. An example is the use of BF_4^- ions (Figure 36) in the self-assembly of tetrahedral cobalt (III) based coordination cages.

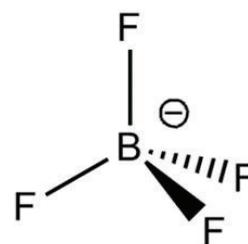


Figure 36 The structure of the BF_4^- anion (Wikiwand, 2020)

The extremely high electronegativity of fluorine causes the boron-fluorine bonds in BF_4^- to become extremely polarised. This means that the large negative dipoles on the fluorine atoms can form strong dipole-dipole electrostatic attractions to the cobalt (III) atoms – ensuring that they form the vertices of the cage – and the positive dipoles on the carbon atoms adjacent to nitrogen atoms in the pyrazolyl-pyridine ligands, ensuring that they form the edges of the cage and act as bridging ligands between to cobalt (III) ions. The tetrahedral geometry of the BF_4^- ion itself ensures that then vertices and edges form in a tetrahedral arrangement so that the final cage structure is tetrahedral (Figure 37).

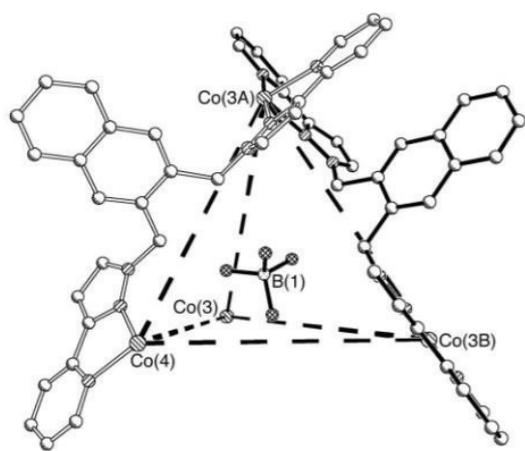


Figure 37 The structure of the BF₄⁻ templated tetrahedral Co(III) cage (Paul, Bell, & Jeffery, 2002)

In face directed templated self-assembly, on the other hand, the templating agents act as the vertices of the cage, and are actually incorporated into the structure of the cage itself, ensuring that the faces of the cage are positioned in the places required to form the desired cage design. An example of a face templated self-assembly is the synthesis of pseudo-tetrahedral Pd₁₂ coordination cages (Figure 38).

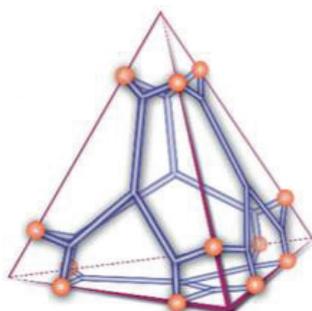


Figure 38 A simplified structure of the pseudo-tetrahedral Pd₁₂ coordination cage (Howlader & Mukherjee, 2016)

The component molecule used as the 'faces' for the cage is [1,3,5-tri(1H-tetrazol-5-yl)benzene] – a symmetrical benzene derivative (Figure 39).

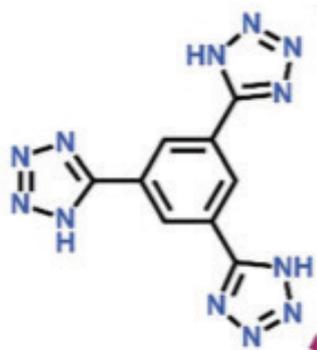


Figure 38 A simplified structure of the pseudo-tetrahedral Pd₁₂ coordination cage (Howlader & Mukherjee, 2016)

The templating agent used is *cis*-(*tmeda*)Pd(NO₃)₂ – a square planar complex of palladium (Figure 40).

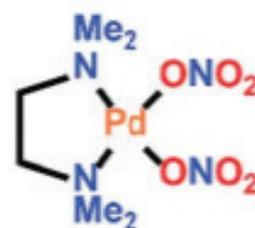


Figure 40 The structure of *cis*-(*tmeda*)Pd(NO₃)₂ (Howlader & Mukherjee, 2016)

During the self-assembly, two of the nitrogen atoms on the five membered heterocyclic rings of the face molecules form dative covalent bonds in ligand substitution reactions with the palladium complexes, and each complex forms such dative covalent bonds with two of the face molecules. The square planar geometry, and the 60° angle that it makes possible, due to the dsp² hybridisation around the palladium (II) atoms, causes the faces to be positioned at exactly the 60° angle required to form a pseudo-tetrahedral structure – specifically a truncated tetrahedron. The palladium (II) atoms form the vertices of the truncated tetrahedron, and their two ligands that are not involved in the cage structure point outside of the cage.

So clearly templating is an incredibly useful technique in self-assembly, because it allows for the formation of very specific cage structures – something that will certainly come in useful in Sections 6,7 and 8 when the applications of supramolecular cages are discussed, for which having the right cage structure is incredibly important.

SECTION 5: WHAT ARE PHOTORELEASE MECHANISMS AND HOW DO THEY WORK?

Release mechanisms refer to the variety of different ways that supramolecular cages, once they have encapsulated a guest, can then be reopened to release the encapsulated guest at the desired time. We have already come across an example of a release mechanism in Section 2 when hemicarcerands were discussed. At high temperatures, the non-covalent interactions between the host and the guest weaken enough for the guest to be released. However, it is extremely difficult to control the temperature of individual host-guest complexes – the temperature distribution of such complexes will follow the Maxwell-Boltzmann distribution. This means that it is extremely difficult to induce opening of hemicarcerands at a specific time and even at temperatures lower than the release temperature, a proportion of the cages will have enough kinetic energy to release the guest, causing release to occur at an unintended time, which, particularly in applications such as drug delivery (Section 8) can have very harmful consequences.

So, if not thermally induced release mechanisms, what mechanisms can be used to induce release of the guest at the desired time and place? It turns out that photorelease mechanisms provide the perfect environment for controllable release mechanisms to successfully occur.

Photorelease mechanisms rely on the interactions between high energy photons and the host-guest complex to alter the binding capabilities of the host. There are two mechanisms by which this can be achieved: photo-induced isomerisation of the cage structure, and photo-induced bond cleavage within the ligands themselves.

The fundamental principle underpinning photo-induced isomerisation

release mechanisms is that when a cage is irradiated with UV light, the irradiation can trigger an intramolecular isomerisation reaction within the ligands themselves. This means that the actual shape of the ligands changes, altering the geometry of the binding sites and hence changing the stability constant for the host-guest complex. If the isomerisation results in a decrease in the stability constant, encapsulation is less energetically favourable than before, so the equilibrium for the encapsulation-decapsulation reaction shifts to increase favourability for the decapsulation reaction, causing a proportion of the host-guest complexes to revert back to individual hosts and guests.

Diethynyl ligands readily perform such photo-induced isomerisation reactions, and so can be used to construct supramolecular cages with such a photorelease mechanism. For example, consider the coordination cage in Figure 41:

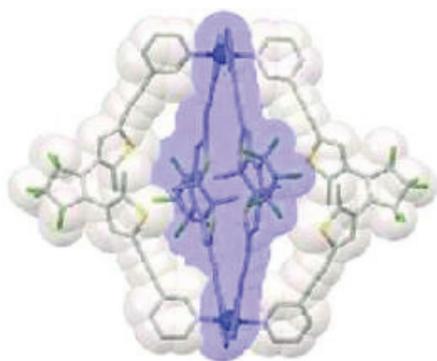


Figure 41 A coordination cage with palladium centres and diethynyl ligands capable of photo-induced isomerisation reactions (Li, Han, Tessarolo, Holstein, & Lübben, 2019)

This coordination cage's geometry rests heavily on the square planar geometry around its two palladium centres (see Section 3) which allows for its four bridging ligands to be arranged parallel to each other, ensuring that the desired geometric change is achieved during the isomerisation reaction. In Figure 42 there is a more in-depth look at the structure of the bridging ligands themselves.

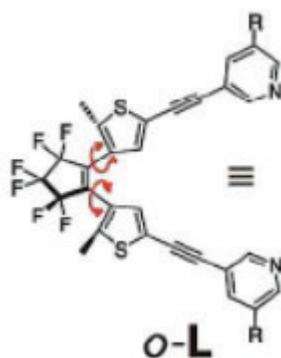


Figure 42 The structure of the open isomer of the bridging ligand (Li, Han, Tessarolo, Holstein, & Lübben, 2019)

The ligands consist of two 3-ethynylpyridine groups bonded to three five-membered rings, two of which are heterocyclic (containing sulphur atoms). Within the ligand there is a large network of conjugated double bonds, which allows degree of delocalisation to occur throughout the molecule. It is likely that this delocalisation is the reason behind the photosensitivity of the molecule, because delocalisation is linked to a number of optical properties of molecules such as colour and light

absorption. These three connected five-membered rings provide an acute angle between the two 3-ethynylpyridine groups, which gives the cage structure a large inner phase – and hence this isomer of the cage is referred to as the open isomer. Having a large inner phase is favourable for encapsulation because it minimises the electron-electron repulsion between the guest and the cage walls by maximising the distance between the guest and the ligands.

When the ligand in Figure 42 is irradiated with 313nm UV light, an isomerism, or more specifically a cyclisation, reaction occurs. The π bonds in the heterocyclic five-membered rings are broken and, via a pericyclic mechanism, a new six-membered ring forms within the region bound by the five-membered rings, forming an isomeric form of the original ligand (Figure 43).

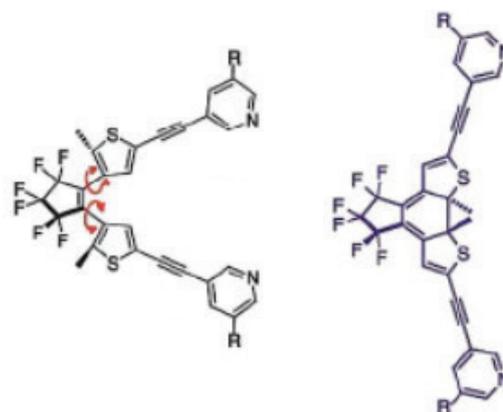


Figure 43 The open form (left) and closed form (right) of the bridging ligands (Li, Han, Tessarolo, Holstein, & Lübben, 2019)

The change in molecular geometry during this cyclisation reaction causes the angle between the two 3-ethynylpyridine groups to become obtuse, causing the inner phase of the cage to become smaller. Hence, this isomer of the cage is referred to as the closed isomer. Curiously, since the two isomers have different conjugated double bond systems, there is an observable colour change for this reaction – the colour changes from yellow to blue as the cage changes from open to closed. This is something that can be detected and used, via colorimetry, to quantify the extent that isomerisation of the open isomer has occurred.

Since the closed isomer of the cage has a much smaller inner phase than the open isomer, there is much greater repulsion between the guest and the cage structure. This makes the encapsulation reaction significantly less energetically favourable for the closed isomer. In experiments conducted by Li et al. in 2019, using a large guest $[B_{12}F_{12}]^{2-}$ (Figure 44) to magnify the repulsion effects, it was found that the change in Gibbs Free Energy for the encapsulation of $[B_{12}F_{12}]^{2-}$ was 40.2% (Li, Han, Tessarolo, Holstein, & Lübben, 2019) higher for the open isomer than the closed one. This may not seem like a great deal, but, since there is a logarithmic relationship between Gibbs Free Energy and the stability constant of the host-guest complex, this 40.2% difference equated to 52.2% of the $[B_{12}F_{12}]^{2-}$ guests being decapsulated and released into the surrounding solution when the open isomer was irradiated with 313nm UV light. So clearly photo-induced isomerism provides a very useful and reliable way of controlling the release of guests from the host cage.

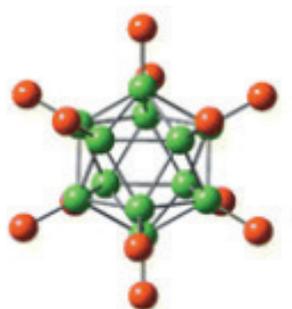


Figure 44 The structure of a [B12F12]²⁻ anion (Balakrishnarajan & Pancharatna, 2015)

Photo-induced isomerism, whilst it may prove to be very successful in many applications of supramolecular cages, poses a problem if biological applications are required – for example, the targeted drug delivery described in Section 8 – because a high intensity of UV light is required to induce a large yield of isomerisation. Such high intensity UV light is likely to be extremely damaging to living cells, making photo-induced isomerism release mechanisms unusable in biological applications. Instead of photo-induced isomerisation, biological applications would require a much more photo-sensitive photorelease mechanism – one that could be triggered using only very low intensity UV light. Photo-induced bond cleavage provides the key to such a release mechanism.

Photo-induced bond cleavage release mechanisms are derived from the principle that UV light can be used to cleave (break) certain chemical bonds. A common example is that, in the presence of UV light, the covalent bond between two chlorine atoms will break homolytically, forming two chlorine radicals (Figure 45).

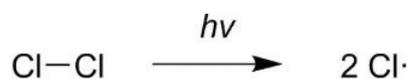


Figure 45 The chemical equation for the photo-induced Cl-Cl bond cleavage to produce two chlorine radicals (Chemistry Stack Exchange, 2016)

In certain circumstances, a bond in a ligand of a supramolecular cage can be cleaved using UV light. This both reduces the binding strength of the host-guest complex, and provides an area, with much less electron repulsion than previously through which the guest can easily escape. The combination of both of these effects means that the cleaving of a bond in one of the ligands can often lead to the guest being released.

An example of such a photo-induced bond cleavage release mechanism was observed by Fang et al. in 2013 in hemicarcerands with nitrophenyl ethers as the bridging ligands (Figure 46). When 330 nm UV light is shone on the hemicarcerands in the presence of water, the bond between the ether oxygen atom and the carbon atom closest to the nitrophenyl group is cleaved, inducing a photochemical oxidation reaction that ends up with the formation of a hydroxyl group and a 2-nitrobenzaldehyde group. The gap created by this cleavage and oxidation process is large enough that the guest can pass through it virtually unhindered and escape the cage.

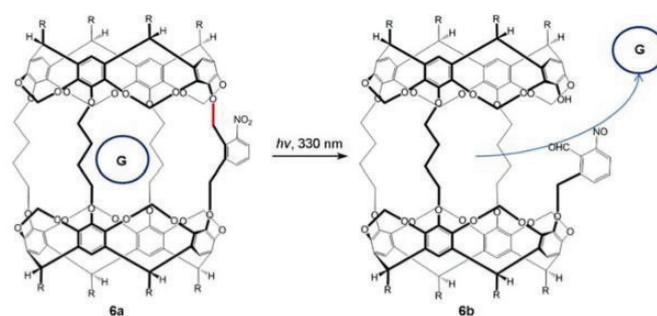


Figure 46 The mechanism for the photo-induced cleavage/oxidation release reaction in hemicarcerands (Fang, Hao, & Houk, 2011)

The exact mechanism for this reaction is still unknown, however, it is believed that it does not involve a free radical mechanism, something that is unusual for chemical reactions involving UV light. Otherwise, we would not expect to see the oxidation products that we obtain – the formation of an aldehyde and a hydroxyl group is much more typical of a form of oxidative cleavage reaction, possibly combined with photo-induced oxidation to form the aldehyde group.

However, the question still stands: why is it only the bond between the ether oxygen atom and the carbon atom closest to the nitrophenyl group that is cleaved and not any other of the bonds in the ligand? The answer to this lies in the dipoles on the respective atoms. The bond between the carbon atom and the oxygen atom is polar – since oxygen is more electronegative than carbon – which creates a large positive dipole on the carbon atom; the other carbon atom also has a positive dipole due to the electron withdrawing effect of the nitro group, but it is a much smaller dipole because of the increased distance between the electron withdrawing nitro group and this carbon. The result is a carbon-carbon single bond in which both carbons have a positive dipole, therefore the repulsion between the carbon atoms will be larger and so, using a bonding model for covalent bonding such as the Lennard-Jones Potential, we can see how this would affect the bond strength. The equation for the Lennard-Jones Potential between two atoms is (ChemGuide, 2019):

$$V(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right)$$

Where V is the potential energy stored in the bond, ϵ is the potential well depth (a measure of how strongly the two particles attract each other), r is the distance between the two bonding atoms and σ is the Van Der Waals radius (the distance at which the potential between the two atoms is zero).

Using this model, we can see that, since there is going to be significant repulsion between the positive dipoles on the two carbon atoms, the value of ϵ is going to be small (since the attraction will be weak). If ϵ is small, it means that the Lennard-Jones potential well is shallow (Figure 47), and so a lower energy is required to overcome the potential well and break the bond compared with normal carbon-carbon bonds. This lower energy requirement means that a larger wavelength (and so lower energy) UV photon can be used to break the carbon-carbon bond. Therefore, if this larger wavelength UV light is used, it will only have enough energy to overcome the potential well and break this carbon-carbon bond; all of the other bonds, due to less repulsion between the bonding atoms, will have much deeper potential wells and so this large wavelength UV light will not have the energy required to overcome the

potential well and break the bond. This means that only the intended bond will break if the correct large wavelength UV light is used for irradiation.

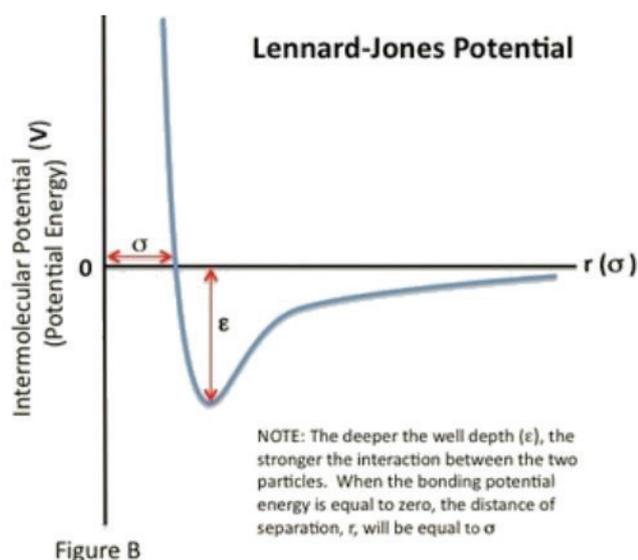


Figure 47 A diagram of the Lennard-Jones Potential illustrating the potential well depth ϵ (ChemGuide, 2019)

However, as well as the wavelength, the type of light source chosen will also play an extremely important role in the success of any photorelease mechanism. There are two main types of light sources that are used for this purpose: flash lamps and two photon excitation.

The flash lamps commonly used for photorelease mechanisms are pulsed xenon-mercury arc lamps. These are gas discharge tubes that rely on the rapid charging and discharging of a gaseous mixture of xenon and mercury to create short flashes of ultraviolet light (Figure 48); the usual time difference between each pulse is 1 millisecond. The mercury atoms are necessary to make sure that UV light is emitted rather than the usual white light produced in arc lamps containing purely xenon.

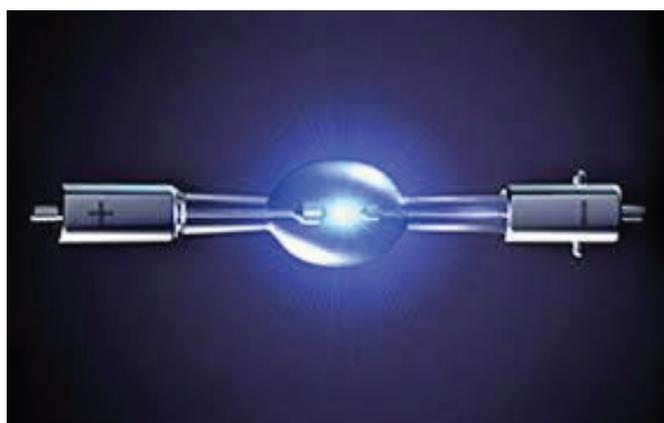


Figure 48 A xenon-mercury arc lamp (Amazon, 2020)

The key advantage of using flash lamps as a source of UV light is that, since the pulse width (the duration of time that photons are being produced) of each flash is longer than most other pulsed UV sources, many rounds of excitation of the same molecule can occur in a single flash, because the excitation time for most organic-based molecules is only a few nanoseconds (much shorter than the pulse width). Moreover, xenon and mercury arc lamps are simple and cheap to make, and

so arc lamps are the irradiation method of choice for almost all applications.

However, xenon and mercury arc lamps pose a large problem if we want to induce photochemical release inside the body. Since the light produced is released in all directions, a large amount of diffraction occurs. As a result, the UV light produced attenuates significantly even just a short distance from the lamp and so the UV light source is not of a high enough intensity to penetrate tissue and so is unable to irradiate and induce photorelease of cages within the body. If we want a UV light source capable of performing such a task, we need to use two photon excitation.

Two photon excitation works on the principle that two relatively low energy photons can be used to excite a fluorophore (usually a sapphire crystal that has been doped with Ti^{3+} ions) and cause it to emit a high energy photon (such as a UV photon) upon deexcitation. The probability (p) of photon release from the fluorophore is governed by the equation (Ellis-Davies, 2007):

$$p \propto \frac{\delta \langle P \rangle^2}{\tau f^2} \left(\frac{NA^2}{2hc\lambda} \right)^2$$

Where δ is the cross-section, $\langle P \rangle$ is the expectation value of the incident power, τ is the pulse width, f is the repetition rate of the incident light, NA is the aperture, λ is the wavelength of light emitted by the fluorophore, and h and c are the Planck constant and the speed of light. This highly non-linear relationship between the probability of release and the other variables means that the stream of photons produced is highly localised in a single direction. As a consequence, two photon excitation can be used to selectively irradiate a highly precise area - such as individual body cells.

Moreover, what makes two photon excitation particularly useful biologically is that, due to the highly localised nature of the UV light produced, little diffraction and attenuation occurs, and so the UV light remains intense enough to penetrate body tissue. Hence, two photon excitation could be used to induce photorelease of cages in specific cells inside the body - something that could be manipulated to create photo-induced targeted drug delivery (Section 9), something that could provide a revolutionary new application for supramolecular cages.

Both photo-induced isomerisation and photo-induced bond cleavage reactions provide effective ways of releasing the guest at the desired time and are extremely useful when devising applications for supramolecular cages (see Sections 6-9). When, however, applications within the body are considered, it is also necessary to consider the intensity of the UV light used, so that damage to tissue does not occur. As a result, for such applications, the use of two photon excitation for photo-induced bond cleavage has shown to be crucial due to its unique ability to precisely penetrate areas of tissue, while remaining at a low, safe intensity.

SECTION 6: CHEMICAL APPLICATIONS OF SUPRAMOLECULAR CAGES

Among the most important applications of supramolecular cages are their chemical applications in areas such as analysis and catalysis. Specifically designed supramolecular cages can act as homogenous catalysts for organic reactions, be used to remove unwanted molecules

from small scale systems, and even solve the problem of observing highly unstable molecules.

One type of supramolecular cage that has the ability to perform a plethora of such applications is coordination cages based on iridium (III) atoms. Iridium (III) is a useful starting material for supramolecular chemists for a number of different reasons. For example, its d^6 electronic structure gives its complexes the same high crystal field splitting energy and stabilisation of the low energy T_{2g} molecular orbital as cobalt (III) (see Section 2), and so iridium (III) complexes are exceptionally stable. Moreover, like some other metals such as mercury, iridium has also been shown to have photosensitisation properties. When iridium atoms are irradiated with light, their molecular orbitals are transferred to an excited state, and when these excited iridium atoms collide with other atoms or molecules, this energy can be transferred to excite other atoms or break bonds. It is this property of iridium that has proven to be crucial in its catalytic properties.

In particular, iridium (III) complexes with tris(4-pyridyl-methyl)-cyclotriguaiacylene (Figure 49) have been shown to have some incredibly useful chemical applications.

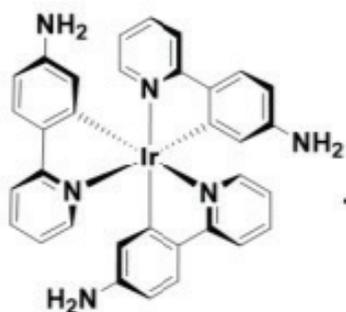


Figure 49 The structure of the iridium (III) complexes with tris(4-pyridyl-methyl)-cyclotriguaiacylene (Rota Martir & Zysman-Colman, 2010)

The complex consists of three bidentate ligands in an octahedral arrangement, and so the chelate effect (Section 2) as well as the high crystal field splitting energy of iridium (III) make this complex extremely stable, and so the cages that it is able to form have very high stability constants.

If this complex reacts in acetonitrile solvent with 2-formylpyridine in the presence of cobalt (II) perchlorate ($\text{Co}(\text{ClO}_4)_2$) – chosen because it readily dissociates to release Co^{2+} ions - a coordination cage with a small inner phase is formed (Figure 50). The cage has a metal ratio (determined by X-ray crystallography) of Ir_2Co_3 .

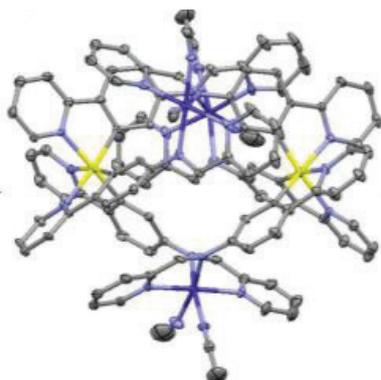


Figure 50 A 3D representation of the iridium (III)/cobalt (III) coordination cage (Rota Martir & Zysman-Colman, 2010)

The cobalt (II) was required to build the cage structure because the tetrahedral geometry of cobalt (II) complexes provided a small bond angle, allowing a cage to form with a small inner phase; the iridium (III) complex, since it is made from bidentate ligands, would provide too shallow a bond angle and so too large a cage would form. Moreover, the cage is made even more stable by the 2-formylpyridine, which dimerises to form bridging ligands to link the transition metal centres. Having bridging ligands, by the chelate effect, ensures that the formation of the coordination cage is entropically favourable and that the cage has a high stability constant.

This iridium-cobalt coordination cage has some very interesting chemical properties. The strong dipole-dipole interactions that can form between the transition metal centres and electronegative elements, such as oxygen, mean that, when the cage is formed in the presence of carbon dioxide (CO_2), the oxidation of carbon dioxide to the carbonate anion (CO_3^{2-}) is catalysed by the iridium (III) complex and the resulting carbonate anion is encapsulated in the cage that forms (Figure 51).

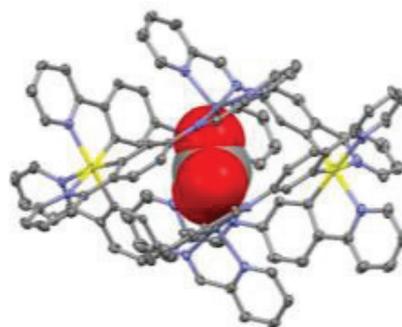


Figure 51 A carbonate anion encapsulated by the iridium (III)/cobalt (III) coordination cage (Rota Martir & Zysman-Colman, 2010)

The same effect is also observed with sulphur dioxide (SO_2), which is oxidised to the sulphite anion (SO_3^{2-}) and encapsulated in the coordination cage (Figure 52).

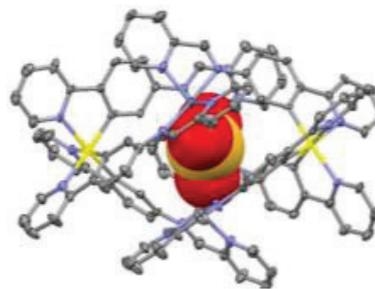


Figure 52 Sulphite anion encapsulated by the Iridium (III)/Cobalt (III) coordination cage (Rota Martir & Zysman-Colman, 2010)

Oxidation reactions such as these are usually extremely difficult and require high temperatures and pressures – the usual way of making sulphite ions involves heating sulphur dioxide with sodium carbonate – and so the fact that the iridium (III)/cobalt (III) coordination cage allows these reactions to occur at room temperature is extremely exciting.

What makes this effect even more remarkable is that the interaction between the transition metal centres and the CO_3^{2-} and SO_3^{2-} , made stronger by the small inner phase size, which reduces the distance over which these non-covalent interactions act, is so strong that encapsulation can even occur once the cage has been formed. Research by Martir and Zysman-Colman showed that when gaseous carbon and sulphur

dioxides were pumped into an acetonitrile solution of the coordination cage, the emission spectrum for the sample changed – the peak intensity at 508 nm was quenched – indicating that encapsulation had occurred.

This extremely high affinity that the coordination cage has for CO₂ and SO₂ has led chemists to postulate that this cage might have an important potential use in the future of removing CO₂ and SO₂ from small scale systems. However, remarkably, this is not even the most exciting use of this coordination cage, Martir and Zysman-Colman also noted that it could be used as a photoactive homogenous catalyst.

The trichloromethylation of 2-ylpyridines (Figure 53) is a reaction that irritated organic chemists for a long time. No matter which mechanism was attempted, the yield was not nearly as high as that of similar reactions.

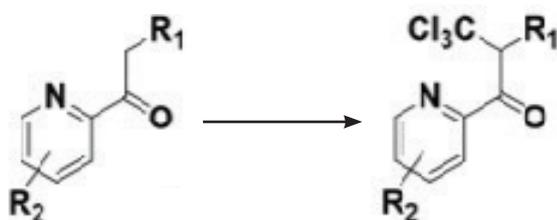


Figure 53 The trichloromethylation of 2-ylpyridines (Rota Martir & Zysman-Colman, 2010)

However, in 2010, it was noted that if the reaction was carried out in acetonitrile solvent and the presence of a 26W fluorescent lamp and the iridium-cobalt coordination cage shown in Figure 50, an extremely high yield was obtained (86-96%) (Rota Martir & Zysman-Colman, 2010).

The exact mechanism is unknown, however, since it only worked in the presence of a 26W fluorescent lamp or other light source, it is believed to involve the photoexcitation of the iridium (III) centres and then, when these centres collide with either reactant, this extra energy can be transferred to them to provide the activation energy required for the reaction. The cobalt (II) centres are also believed to play a part in the catalysis process. The close environment that the cage allows means that both of the catalytic transition metal centres are always close to each other in a rigid platform, increasing the effective reaction concentration within the immediate environment of the reactants, thus increasing the yield.

The theory that the mechanism revolves around the photosensitisation of iridium (III) centres was further strengthened by the fact that this catalysis only works if the coordination cage is empty – because if there is a guest inside, the excited state on the iridium would be transferred to the guest rather than to the reactants (since a collision within a host-guest complex is much more likely to occur) and so the reactants would not receive any energetic benefit from the catalyst.

Another problem that supramolecular cages helped to solve was the problem of observing cyclobutadiene (C₄H₄). Cyclobutadiene has extremely high ring strain - the intended bond angle for its sp² hybridisation is 120°, but the actual bond angles in molecule are close to 90°. This high ring strain makes cyclobutadiene extremely chemically unstable, and so virtually as soon as it is produced, it dimerises in a Diels-Alder reaction, followed by isomerisation, to form the much more stable cyclooctatetraene (Figure 54).

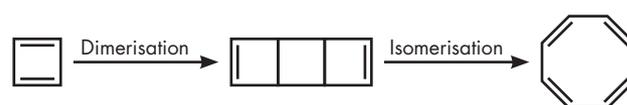


Figure 54 The dimerisation/isomerisation reaction of cyclobutadiene (Ashenhurst, 2020) (Weininger, 2015)

This chemical instability made it extremely difficult to analyse cyclobutadiene spectroscopically, and it required the use of argon matrix isolation techniques to finally isolate it. However, in the 1990s, Donald Cram proposed a much simpler method of isolating cyclobutadiene. If the cyclobutadiene were synthesised within a hemicarcerand (by encapsulating the reactants used to synthesise it) at a low temperature – so that the cyclobutadiene molecules do not have enough energy to escape the cage – the hemicarcerand would prevent the entry of other cyclobutadiene molecules and so the unwanted dimerisation/isomerisation reaction would not be able to occur.

Cram's simple method was shown to be correct using ¹H-NMR spectroscopy. When such spectroscopy was carried out on the proposed encapsulated cyclobutadiene, a sharp singlet was detected on the NMR spectrum at δ_H = 2.27 ppm. This exactly matched the δ_H value obtained for cyclobutadiene using the complicated argon matrix isolation method.

This ground breaking discovery shows the unique ability of supramolecular cages to easily protect reactive or chemically unstable molecules, providing a unique way of analysing them. This ability to protect the guest molecules would also prove to be instrumental in the development of the drug delivery of chemically unstable drugs (Section 8).

So clearly the chemical applications of supramolecular chemistry are incredibly important. The unique reaction environment that coordination cages make possible allows for a whole host of catalytic properties, making difficult reactions, such as the trichloromethylation of 2-ylpyridines, much more viable. Furthermore, their ability to prevent unwanted collisions between reactants allows for notoriously unstable molecules, such as cyclobutadiene, once encapsulated, to be analysed spectroscopically – making them an invaluable tool in analytical chemistry.

SECTION 7: APPLICATIONS OF SUPRAMOLECULAR CAGES TO MOLECULAR SENSORS

Molecular sensors present some of the most exciting and important applications of supramolecular cages, with such diverse applications as toxicology and counter-terrorism. But before looking into how supramolecular cages can be used to design molecular sensors, it is important to first get an idea of what actually constitutes a molecular sensor.

A sensor is defined by John Zhang, a Professor at Dartmouth University and one of the leading experts in molecular sensors, as 'An interface that receives and translates information across physical, chemical or biological domains' (Zhang & Hoshino, 2014). Sensors detect a change in their surroundings and convert that change into a signal that can be detected. Molecular sensors, specifically, detect changes in chemical quantities at an extremely small scale, such as the presence of

a certain toxic molecule, or the concentration of a particular metal ion.

There are three stages in the mechanism of a molecular sensor: Capture and recognition, transduction, and measurement and analysis. Each of these is an integral component to the functionality of the sensor and constitutes a different stage in the sensing process.

Capture and recognition, in its basic form, is the detection of the desired change. In molecular sensors, this is usually achieved by using a signal triggering molecule called a ligand (not to be confused with the ligands used in coordination cages). When the target molecule or ion binds to the ligand, a sensing effect is induced i.e. there is a physical or chemical change to the ligand. This physical or chemical change can then be converted into a signal by a transducer. There are a number of different ways to maximise the effectiveness of the capture and recognition process. One such way is selectivity – the change to the physical or chemical properties of the ligand only occurs when the target molecule binds to it. This is usually achieved by having a very specific binding site on the molecular sensor with complementary electronic structure to the target molecule so that only the target molecule binds strongly enough to the sensor to induce a sensing effect. Sensitivity is also important – a large sensing effect should be generated from few target molecules, meaning that a large, detectable signal can be produced by the transducer; as is dynamic range - the sensing effect should not be saturated by a large number or high concentration of target molecules, allowing for accurate detection of high concentrations of the target molecule.

Transduction is the conversion of the sensing effect into something that can be measured externally. There are a number of ways in which this can be achieved, from producing an electrical signal that can be detected using cyclic voltammetry, to emitting photons of a particular frequency, to causing a change in the UV spectroscopic properties of the sensor. The more sensitive the transducer, i.e. the larger the signal produced from the sensing effect, the easier the signal is to measure, and so the more effective the transducer.

Measurement and analysis is the external interpretation of the signal from the transducer, converting the signal, such as a photon emission, into the desired quantity such as concentration of the target molecule. Computational analysis of the signal data and quantitative analytical techniques such as UV spectroscopy and cyclic voltammetry are incredibly useful in ensuring the effectiveness of the measurement and analysis process.

It may come as no surprise, but in fact the most complex molecular sensors known are those found in nature. Such biological molecular sensors are vastly more intricate and effective than any artificial sensors that have been made. One such example of a biological molecular sensor is the animal olfactory system – for which the discovery of its mechanism was awarded the 2004 Nobel Prize in Physiology and Medicine.

The animal olfactory system (Figure 55) governs an animal's sense of smell and is a complicated network of over 1000 types molecular sensors (called receptors). Each receptor has a different binding site, complementary in electronic structure to over 1000 common odorants (very small organic molecules less than 400 Da in size – usually small ketones and aromatic molecules). When such an odorant enters the nasal cavity it binds to the complementary receptor. Once it has done so, the chemical properties of the olfactory membrane in that area

alter producing an electronic signal, which is transmitted via nerve cells to the brain, where the signal is interpreted and converted into the sensation commonly known as smell.

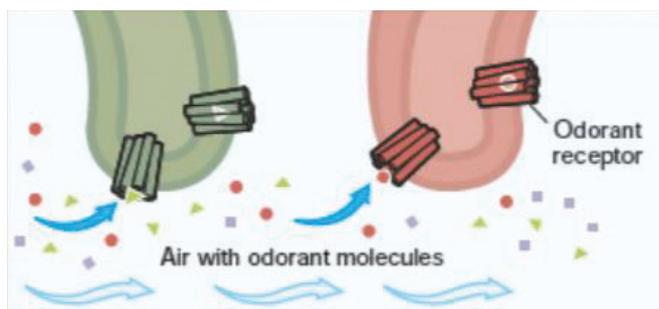


Figure 5 A diagram illustrating the function of molecular sensors in the animal olfactory system (Nobel Prize, 2004)

The result of this sophisticated molecular sensing process is that the nose can detect more than 1000 different 'smells' and, since only one receptor needs to bind to an odorant to produce a signal, the olfactory system can detect extremely low concentrations of odorants.

Whereas molecular sensors designed using supramolecular cages are nowhere near as sophisticated as the animal olfactory system, they nonetheless have a wide variety of different applications. Such molecular sensors based on supramolecular cages can be divided based on the signal that they produce: electrochemical and optical.

Electrochemical molecular sensors are made by attaching a redox active group to the desired receptor. Such redox active groups include ferrocene, quinine and bipyridinium. Supramolecular cages provide the perfect role to act as the receptor because, only guests that can form sufficiently strong non-covalent interactions with the inner phase of the cage can be encapsulated, providing a much desired degree of selectivity to the molecular sensors. However, only coordination cages, cryptands, and to some extent hemicarcerands are applicable to molecular sensors, because the cage must have the ability to encapsulate the target molecules after assembly – cages such as carcerands, from which the guest cannot escape once the cage is assembled are useless because such cages would not allow the target molecule into the inner phase to be encapsulated.

Furthermore, the binding process must be coupled to the redox active group – i.e. the encapsulation process must cause a change in the electrochemical properties of the redox active group. This can be achieved in four main ways. It is worth noting that a number of the examples used contain crown ethers as the binding site, which are macrocycles rather than supramolecular cages. This is because most of the supramolecular molecular sensors research has been directed towards crown ethers, however, crown ethers are very closely related to supramolecular cages, especially cryptands, so the same mechanisms can be applied to both.

1. Through space

Once the target molecule has been encapsulated, there is an electrostatic attraction between the redox active group and the encapsulated target molecule. This alters the electron distribution around the redox active group and so alters its electrochemical properties (Figure 56).

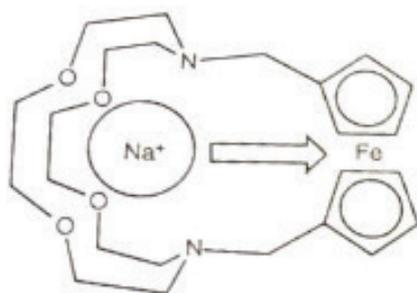


Figure 56 A diagram illustrating a through space interaction in a cryptand based electrochemical molecular sensor (Beer, Gale, & Smith, 1999)

2. Through bond

If the receptor is connected to the redox active group by a conjugated linking group, such as an allyl or benzyl system, upon encapsulation, the electron distribution in the linking group can change, particularly if the encapsulated target molecule is an ion. This change in the electron distribution of the surrounding conjugated linking group alters the electrochemical properties of the redox active group (Figure 57).

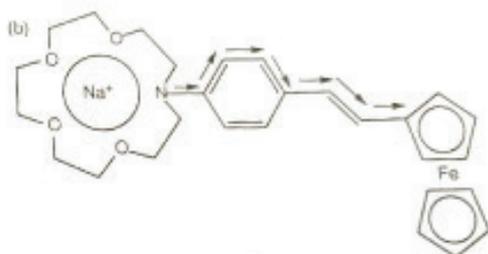


Figure 57 A diagram illustrating a through bond interaction in a crown ether based electrochemical molecular sensor (Beer, Gale, & Smith, 1999)

3. Direct coordination

If the redox active groups are positioned close to the binding site of the target molecule, a coordinate bond can form between the target molecule and the redox active groups, dramatically changing their electrochemical properties (Figure 58).

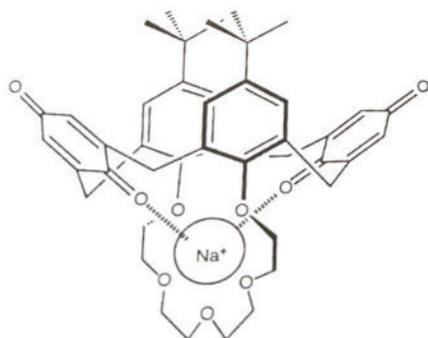


Figure 58 A diagram illustrating a direct coordination interaction in a crown ether based electrochemical molecular sensor (Beer, Gale, & Smith, 1999)

4. Conformational change

In certain circumstances, particularly when bipyridinium is the redox active group, the encapsulation of the target molecule can cause a conformational perturbation of the redox centre, hugely altering its electrochemical properties. For example, when a Ba²⁺ ion is encapsulated in the molecular sensor in Figure 59, the bipyridinium

group rotates, causing its electrochemical properties to change, which can then be detected.

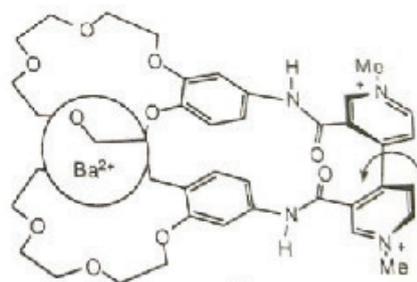


Figure 59 A diagram illustrating conformational change in a crown ether based electrochemical molecular sensor (Beer, Gale, & Smith, 1999)

But the question stands - how can this change in electrochemical activity of the redox active group be quantified and be converted into the desired quantity? Supramolecular chemists use an analytical technique used as cyclic voltammetry to quantify such changes. Cyclic voltammetry involves carrying out the reaction in an electrochemical cell and measuring the current produced at different potentials before and after the reaction. The result is a characteristic 'duck-shaped' graph known as a cyclic voltammogram (Figure 60).

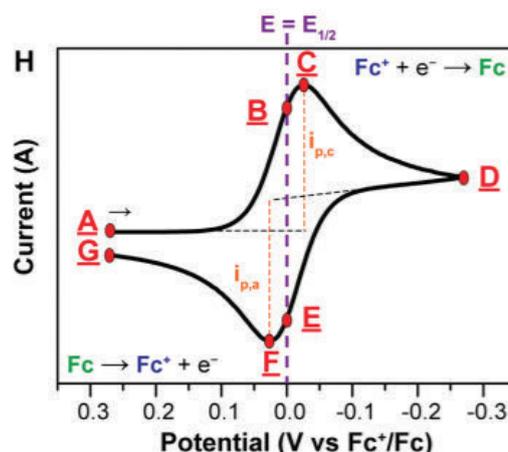


Figure 60 An example of a cyclic voltammogram, with its characteristic 'duck' shape (Elgrishi & Rountree, 2017)

For electrochemical molecular sensors, a change in electrochemical properties of the redox active group will cause a change in the variation of current with voltage before and after the reaction, forming the desired cyclic voltammogram, and then, using a modified form of the Nernst Equation (Elgrishi & Rountree, 2017):

$$E = E^0 + 2.3026 \frac{RT}{nF} \log \left(\frac{[Ox]}{[Red]} \right)$$

Where, E is the standard potential of the species, E⁰ is the relative activity of the oxidised (Ox) and reduced (Red) species, R is the universal gas constant, T is temperature, n is the number of electrons and F is Faraday's constant, the positions of the peaks can be predicted, making it possible to determine the concentrations of the target molecule that caused the change in electrochemical activity.

A particularly useful example of an electrochemical molecular sensor based on a supramolecular cage is the cobalt (III) centred coordination cage in Figure 61, which is used in toxicology to detect the presence and concentration of Cl⁻ ions.

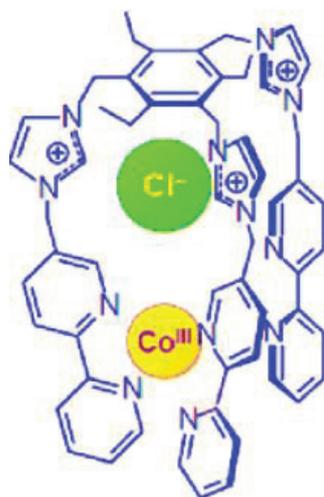


Figure 61 The structure of the cobalt (III) coordination cage used as a molecular sensor for Cl^- ions (Amendola, Boiocchi, & Fabbrizzi, 2008)

In the presence of Cl^- ions, the cage encapsulates one of them; this changes the electrochemical properties of the redox active imidazolium ligands - something that can be detected using cyclic voltammetry (Figure 62) and thereby used to measure the exact concentration of Cl^- .

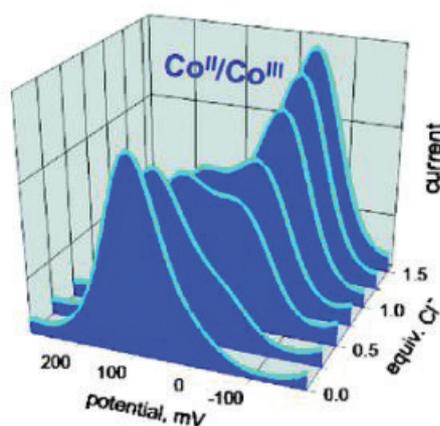


Figure 62 A cyclic voltammogram showing the variation in redox activity of the cobalt (III) coordination cage as the equivalent concentration of Cl^- increases (Amendola, Boiocchi, & Fabbrizzi, 2008)

For optical molecular sensors, the binding site is combined with a fluorophore – a group that emits light upon excitation – rather than a redox active group. The coupling between the binding site and the fluorophore upon encapsulation leads to a measurable emission of photons. This photon emission makes optical molecular sensors extremely useful, because photon emissions are easy to detect, even at very low concentrations, which makes these sensors incredibly sensitive.

An example of such a molecular sensor is shown in Figure 63. When the Na^+ ion guest forms a host-guest complex with the crown ether binding site, the charge on the Na^+ ion alters the electric charge experienced by the fluorophore groups. This changes the wavelength and intensity of the sensor's fluorescence, both of which can be detected and used to quantify the concentration of Na^+ ions.

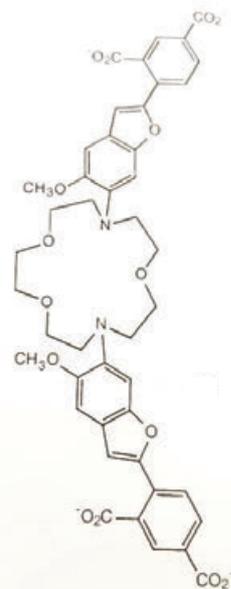


Figure 63 A crown ether based optical molecular sensor used to detect Na^+ ions (Beer, Gale, & Smith, 1999)

This molecular sensor is commonly used to monitor physiological levels of Na^+ ions. It is popular for this purpose because its esterified form is sufficiently water soluble that it can pass through cell membranes, and so can measure Na^+ ion concentration within cells.

However, one of the most exciting and interesting uses of optical molecular sensors is in fact in counter-terrorism. Molecular sensors based on amine supramolecular cages can be used to detect the presence of explosives such as picric acid (Figure 64).

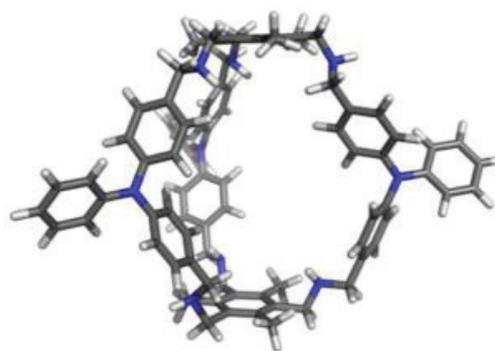


Figure 64 A 3D representation of the amine supramolecular cage based optical molecular sensor (Zwijnenburg, Berardo, Peveler, & Jelfs, 2016)

The amine supramolecular cage has three ligands in a triangular arrangement with a complementary electronic character and perfect orientation to encapsulate picric acid. As a result, picric acid binds very strongly and exclusively to this supramolecular cage. The ligands contain triphenylamine groups, which are strongly fluorescent, and so, upon binding of picric acid, the coupling between the picric acid and the triphenylamine groups causes the fluorescence to occur at a lower intensity and longer wavelength in a process called fluorescent quenching. These changes to the fluorescence can then be detected to show the presence of picric acid.

It turns out that there are two mechanisms that are happening at the same time with the same results that cause this fluorescent quenching – energy transfer and electron transfer.



In the energy transfer mechanism, a real or virtual photon is transferred from a fluorescent triphenylamine group to the picric acid, causing the promotion of an electron from picric acid's HOMO (highest occupied molecular orbital) to its LUMO (lowest unoccupied molecular orbital) in a so called Forster Resonance Energy Transfer (Figure 65).

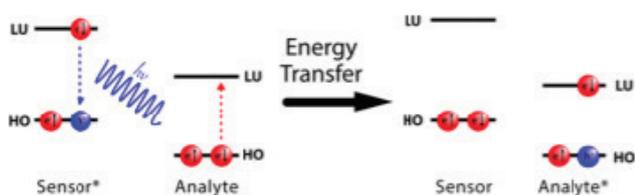


Figure 65 A diagram illustrating Förster Resonance Energy Transfer (Zwijnenburg, Berardo, Peveler, & Jelfs, 2016)

This means that the picric acid is in an excited state rather than the triphenylamine groups, and so the picric acid emits a photon rather than the triphenylamine groups. Picric acid, due to its chemical structure, emits a photon with a much longer wavelength than the triphenylamine groups, hence an increase in wavelength is detected upon encapsulation of picric acid.

In the electron transfer mechanism, an electron is transferred via Photoinduced Electron Transfer (Figure 66) from a triphenylamine group to the picric acid - the triphenylamine group essentially reduces the picric acid. This means that the excited state of the triphenylamine group is converted into a charge separated state with excess electron density on the picric acid. Therefore, the triphenylamine group cannot emit a photon without significant thermal activation - so fluorescence from the triphenylamine groups stops.

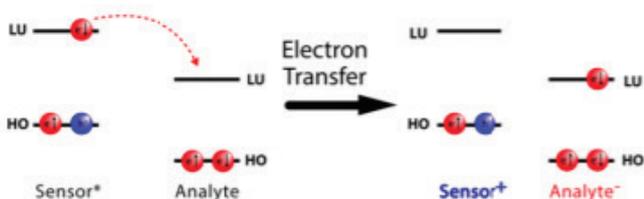


Figure 66 A diagram illustrating Photoinduced Electron Transfer (Zwijnenburg, Berardo, Peveler, & Jelfs, 2016)

The combination of these effects means that only the photons produced from the picric acid are emitted (explaining the change in wavelength observed) and the intensity decreases because the triphenylamine groups are no longer fluorescing.

This remarkable technology is in its early stages, but still provides an exciting step in the fight against terrorism. In fact, it has also been shown that, by replacing the secondary amines with tertiary amines in the cage structure, it is possible to make the binding sites of the cage able to produce the same effect with other common explosives that are similar in structure to picric acid, such as TNT.

Supramolecular cages provide a whole host of new, exciting opportunities when they are applied to molecular sensor technologies. This is a still-emerging field, and yet has already yielded some extremely important discoveries. There seems to be a bright future for supramolecular cages in the field of molecular sensors.

SECTION 8: APPLICATION OF SUPRAMOLECULAR CAGES TO DRUG DELIVERY

Safe, efficient drug delivery is one of the holy grails of pharmacology. If drug delivery systems could be designed that only released the drug in the desired cells, or protected chemically unstable drugs from metabolism, the benefits to patients would be enormous. Although it is still a rapidly emerging field, it is believed that, by using supramolecular cages in drug delivery, both of these outcomes, as well as many more, are possible. In fact, it already seems like supramolecular cages have revolutionised drug delivery by making targeted delivery possible.

Targeted drug delivery is when, although the drug may be taken orally or injected into a vein, the drug lies dormant and does not affect anything until it reaches the intended cells. This may seem impossible, but supramolecular cages allow a way to achieve this impossible task. If the drug is encapsulated in a supramolecular cage that contains a release mechanism (such as those described in Section 5), whilst the release mechanism is not triggered, the drug is protected from other molecules that could react with it and deactivate it, and the drug cannot escape the supramolecular cage, meaning that it cannot affect any unintended areas. However, once the encapsulated drug reaches the intended cells, the release mechanism is triggered, causing the cage to open and the drug to be released. This ensures that the drug can only affect the intended cells.

This use of supramolecular cages for targeted delivery provides an incredibly effective solution to three of the biggest problems faced by drug delivery mechanisms: cross-reactivity, metabolism and unintended cell death.

Cross-reactivity refers to the biological phenomenon by which molecules with similar structures to known antigens can trigger an immune response. The antibodies that are complementary to the antigen are always present in the bloodstream, so when the molecule with a similar chemical structure enters the blood stream, the antibodies can bind to that molecule. This binding process triggers an immune response, which may be as mild as a slightly heightened temperature, but could be as serious as anaphylaxis, which can often be fatal. This poses problems with a number of medications. For example, patients who have sulphite allergies have been shown to have a serious, and often deadly, immune response when administered the drugs sulphasalazine (a prostaglandin inhibitor used to treat rheumatoid arthritis) or sulphamethoxazole (an antibiotic used to treat urinary tract infections and E.coli) due to the structural similarities between the sulphite ion and the sulphonyl groups on the two drugs (Figure 67).

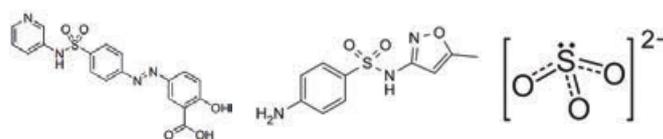


Figure 67 The structures of (left to right): sulphasalazine, sulphamethoxazole and the sulphite anion (Pfizer, 2020), (Catclock, 2013), (Neurotiker, 2008)

In a non-pharmaceutical context, the similarities in the hevein protein structures in latex and bananas mean that cross-reactivity can occur, meaning that many people who suffer from a latex allergy also suffer an allergic reaction to bananas.



The targeted delivery made possible by supramolecular cages would solve the issue of cross-reactivity. In the case of sulphasalazine, if the drug were encapsulated in a supramolecular cage before being administered, it would no longer be able to bind with the sulphite antibodies while in the bloodstream and so no immune response would occur. Once the encapsulated sulphasalazine had passed into the desired cells, the release mechanisms could be triggered, releasing the sulphasalazine, causing the intended prostaglandin inhibiting effects without an immune response.

Some drugs are particularly sensitive to metabolism - the biological process of breaking down large molecules that occurs predominately in the liver. Moreover, for some drugs, metabolism can have some extremely deadly and sometimes fatal consequences. An example of such a drug is the anti-inflammatory drug tienilic acid (Figure 68), which can be used to treat hypertension.

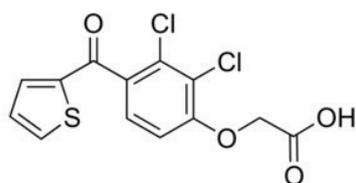


Figure 68 The structure of tienilic acid (Sigma Aldrich, 2020)

Tienilic acid was withdrawn by SmithKline, its manufacturer after only three years of being on the market, due to the discovery that once metabolised, the drug transformed into powerful toxins, killing many of the patients who were prescribed the drug. The situation was so severe that criminal charges were brought against SmithKline for misbranding and hiding data related to the toxicity of the drug. So, what exactly was the problem with tienilic acid?

When tienilic acid is administered, it enters the blood stream and passes through the liver. Most drugs are unaffected by the liver and simply pass through on their way to their target cells, however, tienilic acid is metabolised by the liver and converted to a thiophene-S-oxide intermediate (Figure 69). This intermediate is extremely toxic because it can bind to, and thereby alter the structure of, hepatocellular proteins, causing extensive cell death within the liver – something which can often prove to be fatal.

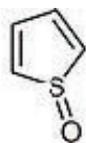


Figure 69 The structure of thiophene-S-oxide (Thiemann, 2018)

Supramolecular cages could prevent a tragedy like that caused by tienilic acid from ever happening again because, if the drug were encapsulated in a supramolecular cage, it would not be able to be metabolised as it passes through the liver – providing the structure of the cage itself was stable enough not to be metabolised, and so it would pass to the target cells in its desired form, where the release mechanism could be triggered, releasing the drug into the cell, allowing the drug to safely cause the desired effects to the intended cells.

Unintended cell death is a large problem with chemotherapy drugs. Many chemotherapy drugs such as fluorouracil (see Section 9) work by

altering the DNA of the cancerous cells, and in doing so, change the protein production in the cell, which causes the cell to die. However, this mechanism does not work solely on cancerous cells – normal, healthy cells also contain DNA and so are affected too and are also killed by the chemotherapy drug. This means that many chemotherapy treatments cause a number of adverse effects as well as treating the cancer – and in many cases do more harm than good. Supramolecular cages, and the targeted release that they allow, could rectify this problem and help to make chemotherapy treatments much safer and more viable.

Cisplatin ($\text{Pt}(\text{NH}_3)_2\text{Cl}_2$), a square planar platinum complex, is such a chemotherapy drug that would benefit from encapsulation in a supramolecular cage. At the moment, cisplatin is used to treat a whole variety of different cancers, including ovarian, cervical, and oesophageal. However, cisplatin is known to cause many serious side effects due to unintended cell death such as nephrotoxicity and neurotoxicity, which in many cases can prove fatal. Woods and Wenzel in 2019 designed a palladium centred coordination cage, using conjugated bidentate bipyridyl ligands, that is capable of encapsulating cisplatin (Figure 70).

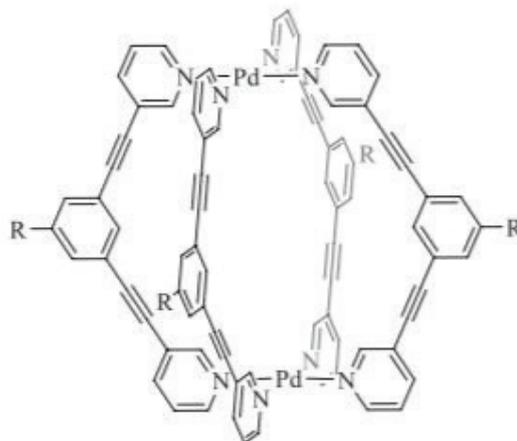


Figure 70 The structure of the coordination cage capable of encapsulating cisplatin designed by Woods and Wenzel (Woods, et al., 2019)

The hydrophobic interior of the cage means that the hydrophobic effect (Section 4) could be used to increase the change in entropy for the encapsulation process, and so increase the stability constant of the host-guest complex formed. Encapsulation of cisplatin in a cage like this would mean that cisplatin would remain inactive until it reached the intended cancerous cells, where a highly localised trigger for the release mechanism, such as two photon excitation (Section 5) or using so called DNA aptamer locks that only open and release the drug in the presence of the mutated DNA, would cause the release of the cisplatin inside only the cancerous cells – ensuring the death of cancerous cells without harming healthy ones. Clearly such targeted release technology that supramolecular cages allow would revolutionise the chemotherapy process.

However, targeted delivery is not the only benefit of using supramolecular cages in drug delivery. Supramolecular cages can also be used to vastly increase the water solubility of drugs. Water solubility is a crucial property for drugs – if drugs are not water soluble, they cannot pass through the cell membrane and access the cell interior, and so are unlikely to work - yet 40% of approved drugs are poorly water soluble (Kalepu & Nekkanti, 2015) and so remain virtually unusable.



If, however, the drug is encapsulated in a water soluble supramolecular cage, such as the iron (III) based coordination cage in Figure 71 developed by Nitschke in 2017, suddenly these drugs are able to access the cell interior by waiting for the encapsulated form to enter the desired cells, and then triggering the release mechanism to release the drug. This application of water soluble supramolecular cages would allow thousands of previously unusable drugs to be used, which would have a vast positive benefit for medical care.

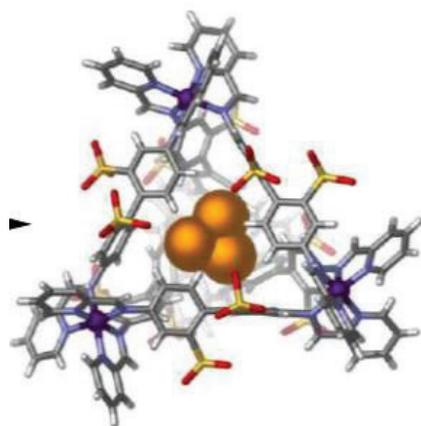


Figure 71 The structure of a water soluble iron (III) centred coordination cage, with an encapsulated P_4 molecule, designed by Nitschke (Georges, 2017)

An example of a drug that such encapsulation with water soluble supramolecular cages would hugely impact is the antibiotic ciprofloxacin, used to treat typhoid fever and bacterial respiratory tract infections (Figure 72).

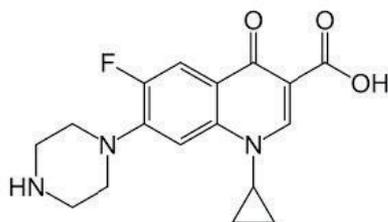


Figure 72 The structure of ciprofloxacin (Fvasconcellos, 2008)

Apart from the one carboxylic acid group, the rest of the ciprofloxacin molecule is very hydrophobic and so it has incredibly low solubility in water. At the moment, ciprofloxacin's solubility is improved by using lactic acid as a pH modifier when it is administered. However, lactic acid is toxic – it is the unwanted by-product of anaerobic respiration – and so can cause cell death and other adverse effects. Encapsulating ciprofloxacin in a water soluble supramolecular cage, such as that in Figure 71, would allow for safer, more effective delivery of the drug and hugely benefit the patients that are prescribed it.

It is clear that supramolecular cages have a phenomenal positive impact on drug delivery. Whilst many of these technologies are not available for clinical trials yet – there are various kinks in solubility and release mechanisms that still need to be worked out. It does not seem like it will be long until supramolecular cages become a regular addition to the administration of a whole variety of drugs.

SECTION 9: DESIGNING A NEW SUPRAMOLECULAR CAGE TO SOLVE THE ISSUES OF FLUOROURACIL AS A CHEMOTHERAPY DRUG

Now that I had researched the many different facets of supramolecular cages and their applications, I thought that it would be a good idea to use the information that I had obtained and apply it to solve a real world problem.

I wanted the problem that I would provide a solution for to be one that would have a large positive impact on society if it were solved. So, it seemed like a natural progression to decide to solve a problem concerning drug delivery - in particular the delivery of chemotherapy drugs – because if safe, targeted delivery of chemotherapy drugs could be obtained, it would hugely benefit countless cancer patients across the globe.

When considering which chemotherapy drug to design a supramolecular cage for, there were a number of criteria that the chosen drug would have to fulfil:

- The drug must have a relatively simple chemical structure.
- The drug must have the ability to form strong non-covalent interactions to counteract the often entropic unfavourability of encapsulation.

Both of these aspects were important due to the limited time frame available for the design, as they both reduce the complexity of the cage required to encapsulate the drug.

In addition:

- The drug must have a high potential, but have large downfalls at the moment, which mean that its current use is limited.

This is particularly important because the chosen drug must actually be one that would benefit from encapsulation – if it were a drug that works perfectly fine without encapsulation, such as paracetamol or ibuprofen, there would be no point in encapsulating it.

In my search to find a chemotherapy drug that satisfied all of these criteria, fluorouracil in particular stood out (Figure 73).

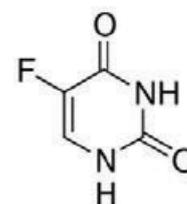


Figure 73 The chemical structure of fluorouracil (Sigma Aldrich, 2020)

Fluorouracil was a perfect drug to be considered for a number of different reasons. Since it was first patented in 1956, fluorouracil has been used as a chemotherapy drug to treat a number of different cancers, such as pancreatic, colorectal and stomach. However, it is now only used in very extreme circumstances, despite being incredibly effective at cancer treatment. This is due to a particularly sinister side effect; fluorouracil, as well as killing the intended cancer cells also kills cells in the cerebellum (the area of the brain that controls balance, coordination and speech). Patients who have been administered fluorouracil have been shown to have an extremely high risk of



developing such debilitating conditions as acute cerebellar syndrome, ataxia, nystagmus and dysmetria.

This means that fluorouracil would greatly benefit from encapsulation, and the targeted release that it would allow. If the cage has a suitable release mechanism, the fluorouracil molecules would only be released once inside the target cells and would remain inactive in all other parts of the body. This means that the damage to the cerebellum would not occur, and so fluorouracil would be able to be used much more extensively – no longer being limited to solely extreme cases.

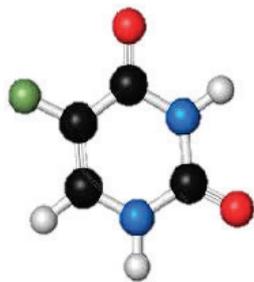


Figure 74 The 3D structure of fluorouracil (Science Photo, 2020)

Furthermore, some properties of fluorouracil's structure make it a perfect drug to be encapsulated. All of the five substituents on the heterocyclic ring can take part in hydrogen bonding, the strongest of the commonly used non-covalent interactions and, in addition, in the pseudo-chair conformer that is most energetically favourable for the molecule to adopt, the fluorine and nitrogen atoms are in the same plane. This is very important because it means that, despite the directionality of hydrogen bonds, a receptor could be designed inside the cage that could allow three strong non-covalent interactions to occur simultaneously. Both the fact that fluorouracil can form hydrogen bonds, and the fact that its conformation allows for multiple strong non-covalent interactions to be formed at the same time means that, with a precisely designed receptor, a cage could be designed for fluorouracil that would release a large amount of energy upon encapsulation, thereby

increasing the stability constant for the interaction and making the host-guest complex more likely to form.

However, the problem with fluorine in a design such as this one is that the non-covalent interaction that it undergoes varies depending on the fluorine atom's environment. When there is low electron density, there is an insufficiently large negative dipole on the fluorine atom to undergo hydrogen bonding, so instead it undergoes an orthogonal multipolar interaction (Figure 75). Conversely, when there is a high electron density around the fluorine atom, it can form a hydrogen bond in the usual tetrahedral geometry (Figure 75). Since these two interactions have completely different molecular geometries, before designing a receptor, it was important to determine which interaction would take place in fluorouracil. To do this, ^{19}F -NMR was used.

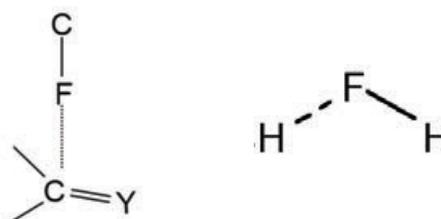


Figure 75 Diagrams showing fluorine atoms participating in a multipolar interaction (left) and hydrogen bonding (right) (Vulpetti, 2013) (Jobilize, 2020)

The principle behind using ^{19}F -NMR is that, if there is a low electron density around the fluorine atom, there will be a smaller opposing magnetic field generated by the fluorine atom, and so the corresponding peak will be at a high chemical shift, and the inverse is true when there is a high electron density around the fluorine atom. Therefore, ^{19}F -NMR provides a good indicator of the electron density around fluorine atoms, and hence the form of non-covalent interaction that they are likely to undergo. The ^{19}F -NMR spectrum for fluorouracil (Figure 76) shows one sharp peak at -171 ppm. This is quite a low chemical shift for a ^{19}F -NMR spectrum, and so indicates that there is a high electron density around the fluorine atom in fluorouracil, and so it will participate in hydrogen bonding rather than an orthogonal multipolar interaction.

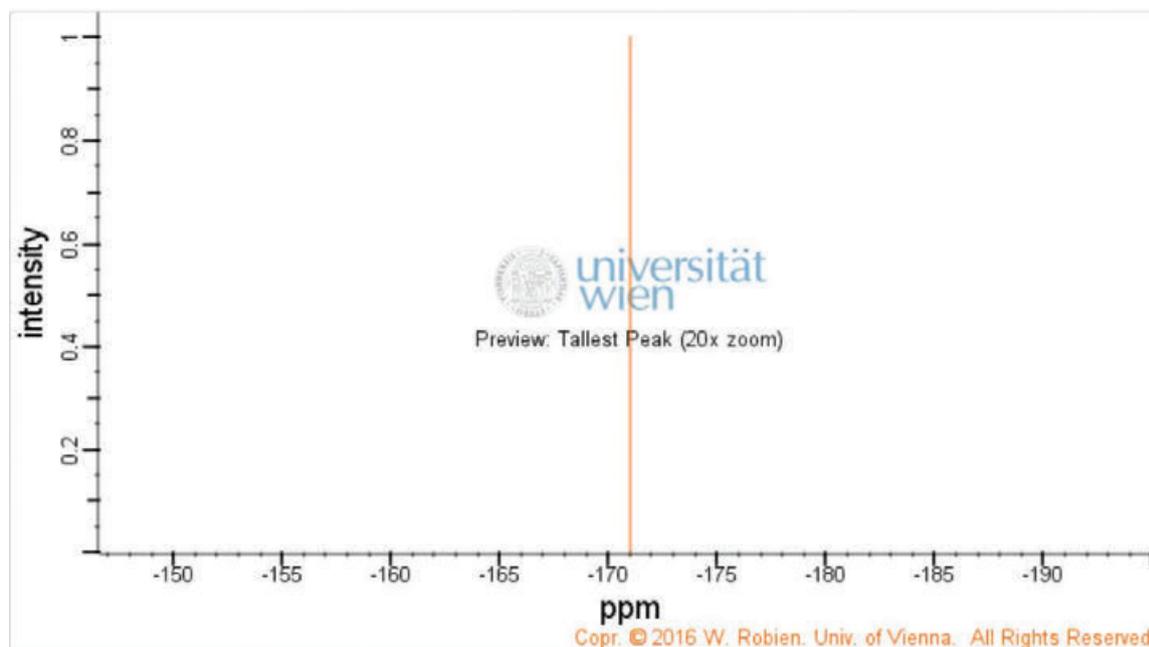


Figure 76 ^{19}F -NMR spectrum for fluorouracil (Robins, 1976)

Now that the guest had been chosen and its non-covalent interactions determined, it was possible to design a receptor that would be able to bind to the guest. The receptor in the cage that I designed consists of three imine groups that form an equilateral triangle and are all in the same horizontal plane.

The position of the imine groups maximises the number of strong non-covalent interactions experienced by the fluorouracil molecule – the N-H groups will form hydrogen bonds with the lone pairs on two of the imine groups, and the fluorine atom will form a hydrogen bond with the hydrogen atom on the other imine group. Since all three hydrogen bonds act with the same directionality, a planar configuration of imine groups in the receptor would allow for all three interactions to occur simultaneously, greatly increasing the energy released upon encapsulation.

Furthermore, there is going to be a repulsion between the carbonyl groups on the fluorouracil molecule and the imine groups in the receptor, so this will make it very energetically unfavourable for the fluorouracil molecules to deviate from the desired arrangement because, not only will it mean weakening the interactions between the molecule and the receptor, but it will also increase the repulsion between the receptor and the molecule. Therefore, the combination of these two effects ensures that the lowest energy configuration, and so the configuration in which the system will spend the majority of its time, is the desired configuration with three strong hydrogen bonds between the fluorouracil molecule and the cage.

Now that the receptor had been designed, it was now necessary to look at the most effective cage design. Straight away it was concluded that having only three edges to the cage at any vertex would be optimal – any more than three would either move the imine groups of the receptor away from their optimal triangular arrangement or increase the repulsion between the carbonyl groups of fluorouracil and the cage, thereby making the desired configuration less stable and so lowering the stability constant for the host-guest complex.

When determining the best type such a cage to use, a tetrahedral coordination cage first came to mind, such as Figure 77, because this is a geometry that is easy to obtain using the tetrahedral geometry of transition metal atoms that form complexes with a coordination number of 4 such as iron (II).

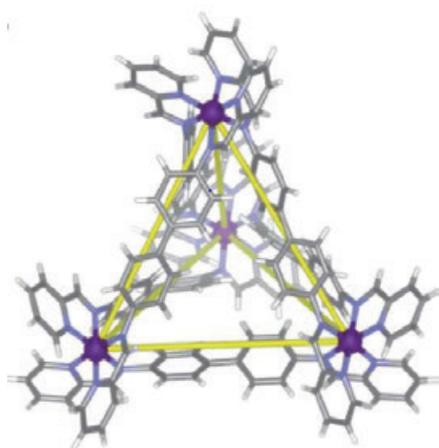


Figure 77 A tetrahedral coordination cage based on iron (II) centres (Nitschke & Clegg, 2013)

However, when considering the geometry of the imine groups of the receptor within such a cage, it became abundantly clear that a tetrahedral geometry would not be suitable. Due to the angle of slope of the edges in a tetrahedron if each imine group is positioned on one of the edges, they will no longer be coplanar, but instead all point towards a common point on the base of the tetrahedron. If the imine groups are no longer coplanar, it means that a fluorouracil molecule will no longer be able to form three simultaneous strong hydrogen bonds, and so the energy released upon encapsulation will be reduced, so the stability constant for the host-guest complex will be much lower.

The only feasible way to counteract this problem would be to use a hexagonal aromatic ring to counteract the slope of the tetrahedron's sides, but imine groups cannot bond to most aromatic rings without breaking the aromaticity and therefore distorting the configuration. As a result, it was decided that a tetrahedral cage would not be the way to go, so instead it was necessary to look for a three edged cage in which the edges were parallel so that the desired coplanar configuration of the imine groups in the receptor could be obtained. Since this would likely require a more unconventional molecular geometry, it was deemed a good idea to narrow the search and focus on coordination cages – the more diverse geometry around transition metal centres seemed more likely to be able yield the desired configuration (as laid out in Section 3).

In the end, the desired geometry was found by using an interesting property of molybdenum. Molybdenum has a coordination number of 6, which would normally lead to an octahedral geometry, however, for certain σ -donor ligands such as $-\text{CH}_3$, it turns out that, if the high energy t_{1u} molecular orbital rehybridises into an a''_2 and an e' molecular orbital, a lower energy and therefore more stable configuration is obtained. This rehybridization changes the point group from O_h to D_{3h} , which changes the geometry around the molybdenum atom from octahedral to trigonal prismatic. If three bidentate ligands (such as dithiolene derivatives) are then bound to this trigonal prismatic molybdenum atom, the end result is three parallel ligands in the desired triangular arrangement that are parallel to each other (Figure 78).

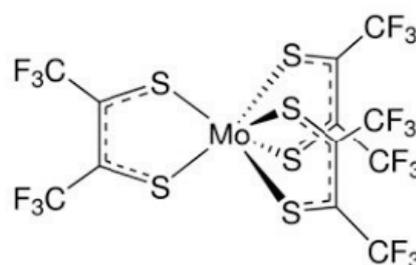


Figure 78 A trigonal prismatic molybdenum-dithiolene complex (Sigma Aldrich, 2020)

By the chelate effect, using bidentate ligands around the molybdenum centre makes the formation of the cage much more entropically favourable, and so the desired cage will be much easier to assemble.

Moreover, if the ligands are used to bridge two molybdenum centres together (in an M_2L_3 cage) not only will the entropic favourability of bridging ligands aid the assembly, but the fact that both centres have a trigonal prismatic geometry will ensure that the that the desired receptor geometry (coplanar imine groups in a triangular arrangement) can easily be achieved in the final cage design.

Molybdenum, unlike some transition metals, is safe to use in the body because it is non-toxic. In fact, molybdenum is vital for the production of four important enzymes: sulphite oxidase, which oxidises sulphites to sulphates; aldehyde oxidase, which oxidises aldehydes to carboxylic acids; xanthine oxidase, which oxidises hypoxanthine to xanthine, and mitochondrial amidoxime reducing component (mARC), which reduces hydroxylated compounds.

With the basic cage design decided, it was now necessary to consider the choice of ligands in more depth. There are two elements that had to be included in the final ligand design. First, the ligands had to be identical and symmetrical – otherwise different isomers of the cage would form; secondly, the ligands must have a dithiolene group at each end to bind to the molybdenum centre.

However, since molybdenum does not have any special optical properties, the key to the release mechanism must lie in the ligands. Since targeted release is key for the function of this supramolecular cage, it was concluded that photorelease would be the most appropriate release mechanism, because the high directionality and tissue penetrating ability of two photon excitation would allow for precise release inside specific cells in the body. In particular, one type of photo-induced bond cleavage reaction studied by Fang (Section 5) stood out as being a particularly interesting example to be considered.

The reaction shows that, when a ligand containing a nitrophenyl ether functional group is irradiated by low intensity 330nm UV light in the presence of water, the oxygen-carbon bond closest to the nitrophenyl group is cleaved in a photo-induced oxidative cleavage/oxidation reaction and the cage opens (see Figure 46 Section 5), allowing the guest to escape. This reaction would be easily applicable to a cell environment due to the high water concentration inside the cell. Moreover, what makes this reaction particularly useful in the context of this supramolecular cage is the fact that the intensity of UV required to induce bond cleavage is extremely low – in fact, ordinary sunlight can induce the photochemical reaction. This means that any cell damage caused by the UV light would be greatly limited.

Two photon excitation, even though it has a far greater penetrating power than any other ultraviolet source, can still only penetrate 1mm of skin. Therefore, if this type of mechanism were to be applied to cancer therapy, it would require a precise surgical insertion of the UV source into the region of cancerous cells, and would be limited to relatively small areas of cancerous tissue.

Therefore, my final design for the ligand draws from this nitrophenyl ether photochemical reaction and incorporates it, along with the other necessary elements (Figure 79). Only one ligand needs to cleave for successful release to occur, so the fact that all three ligands contain a nitrophenyl ether group triples the probability that the fluorouracil molecule will be successfully released.

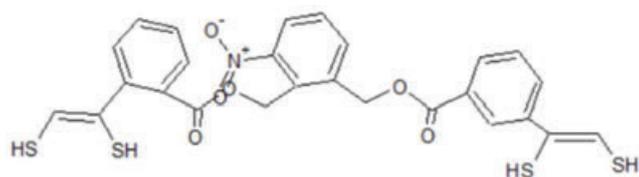


Figure 79 The structure of the bidentate chelating ligand that I designed for the supramolecular cage

Importantly, to conserve symmetry, each ligand has two imine groups, meaning that each cage has the capability of encapsulating two fluorouracil molecules at any one time. The billiard ball effect described in Section 2 is unlikely to occur because the strength of the non-covalent interactions at each receptor will restrict the movement of each fluorouracil molecule, making a high energy collision unlikely. Therefore, when calculating the stability constant for this cage, it would be necessary to use the exact formula derived in Section 1 and take the sum from $n=1$ to $n=2$. Furthermore, the complementary electronic nature of the receptor to fluorouracil means that the strong non-covalent interactions between fluorouracil and the imine groups on the ligands could help to template the assembly of the cage – making the assembly process much more viable.

The final element of the cage design to consider is solubility. In order for the cage to pass into cells and achieve its function, it is paramount that it is soluble in water. Therefore, to rectify this issue, short polyethylene glycol (PEG_{short}) groups were bonded to each dithiolene group. PEG_{short} groups are extremely hydrophilic, and so should easily solvate the cage.

Now a design had been finalised for the cage to encapsulate fluorouracil (Figure 80). The mechanism for the drug delivery would occur in the following way: The cage would be assembled in the presence of a high concentration of fluorouracil, and the fluorouracil molecules will be encapsulated as the cage is assembled. The encapsulated fluorouracil would then be administered into the body where it would pass through the cell membranes (due to the cage's water solubility) into cells, including the cancerous cells. Directed two photon excitation would precisely target low intensity UV light to the cancerous cells, so the only cages to open would be the ones in the cancerous cells. Therefore, only the desired, cancerous cells would be killed by the fluorouracil. All of the other non-released cages would simply be excreted from the body over time and remain unopened, so no healthy cells would be harmed.

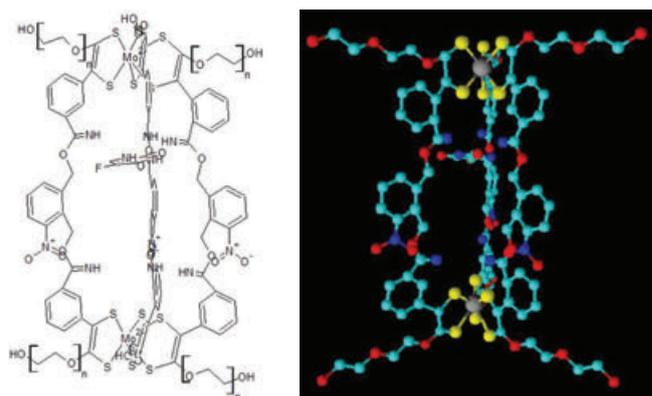


Figure 80 The 3D representation and structure of my final cage design with a fluorouracil molecule encapsulated

Supramolecular cages are clearly going to be hugely important in the development of safe, effective chemotherapy drugs. Whilst the supramolecular cage that I designed is far from a complete solution to the problem – there will doubtless be a whole host of problems in the assembly process that would have to be overcome – the design is the first step in the journey towards a successful end result. Who knows – maybe in the future, molybdenum coordination cages may become important in drug delivery of chemotherapy drugs, or maybe there is a new breakthrough just beyond the horizon that will be discovered in years to come?



Pot Luck Politicians: A Parliamentary Chamber from Sortition

Tom Welsh

CHAPTER 1: INTRODUCTION

"It is accepted as democratic when public offices are allocated by lot; and as oligarchic when they are filled by elections"

Aristotle's Politics (Book IV)

This paper seeks to outline the theoretical and practical benefits associated with the potential application of sortition within the political system of the United Kingdom. Sortition is, in effect, the selection of individuals by random lottery, and can in this instance be seen as a sort of political jury service whereby a group of individuals representative of the population as a whole are asked to vote in the legislative process as to whether they agree with the intentions and /or methods behind proposed laws. Whilst appearing initially ill thought through or novel it will be shown to be neither, with both extensive historical use in ancient, medieval, and to a lesser extent, modern Europe. Furthermore, sortition has long been described in classical political theory as the purest form of democracy on the basis of its equality and representativeness. The case will be also then be made as to why specifically the United Kingdom is apt to benefit from sortition's implementation as a consequence of its current political state of affairs, and then additionally as to in what way sortition might be worked into the existing legislative framework to best effect.

CHAPTER 2: HISTORY AND THEORY OF SORTITION

"Even foolish men would rather govern themselves than be governed by others"

Thomas Hobbes' Leviathan (Chapter XV)

2.1: HISTORICAL USE OF SORTITION

It is fair to say that both the utilisation of sortition within political systems has waxed and waned over the course of the last two-and-a-half millennia and that there has been a recent uptake of interest in sortition within academia in the last fifty years or so. Nonetheless an appreciation of how sortition has been applied historically, often to immense success, is useful in order to objectively evaluate the likelihood of its application in the UK Parliament of today being a beneficial one.

2.1.1: CLASSICAL ATHENS

First being used in the 6th century BC, sortition was integral to Athenian democracy. Fundamentally its use arose out of the desire for each citizen to receive equality of legal and political rights; as such sortition was implemented in both the selection of legal juries and the Athenian Council. The Athenians operated a system whereby individuals had bronze cards with their names on which were then inserted into slots on

a machine called a 'kleroterion' (which is pictured on the cover page of this paper). A row or column was then selected at random and the individuals whose cards were in that sample were selected. It is to be noted that the qualification for eligibility was limited to male Athenians over thirty, with: women, slaves, younger men and foreigners excluded. The Council was composed of 500 administrators and was responsible for developing legislation; overseeing the executive; and managing diplomacy. Each individual selected served a one-year term and it is estimated that 50-70% of all men eligible had served at least one term; this being possible due to the population of Athens being only in the tens of thousands during the period.

The Greeks argued that selection by lot was the most democratic method as it gave even the most unpopular an equal chance of selection – yet it was never the sole method used for the appointment of positions. Military commanders, for example, were not chosen by sortition with instead a man's military capabilities the determining factor behind choice. This recognition of the importance of expertise in leadership, even if not directly political leadership, has been a key factor of consideration ever since.

Beyond its equitable treatment of people, sortition was also highly regarded for its ability to prevent factionalism. As power was diluted given the size of the Council, and each member was selected not on the basis of their desire for power but their eligibility, collusion became rare. As the classical historian James Headlam-Morley wrote in his 1891 book *On Election by Lot at Athens*, "systematic oppression and organised fraud were impossible". That is not to say that the situation was perfect, with the occasional levying of too high taxes being a problem: then again, to expect any political system to never make mistakes is perhaps to be asking too much. Indeed it shall be later seen in this paper that many philosophers of the time took great dislike to sortition, and Athenian democracy more broadly.

2.1.2: MEDIEVAL AND MODERN PERIODS

Alongside the adoption of classical culture in the Renaissance came the re-emergence of sortition. Bologna, Parma, and Vincenza all used random selection of legislators. Moreover, sortition was also used in Florence during the 13th and 14th centuries, and in Venice from 1268 until the Venetian Republic fell in 1797 where sortition played a notably key role in the selection of the Doge. The Kingdom of Aragon utilised sortition too with Ferdinand II extolling its virtues.

For an example of even more recent application one can look to San Marino where sortition was used until the end of the Second World War. San Marino used to randomly select its two Heads of State from its sixty councillors; a not insignificant fraction of its minute population. Even more recently Iceland, following its 2008-2011 financial crisis,



assembled a committee of 950 citizens to provide advice on the development of a new constitution.

2.2: SORTITION WITHIN POLITICAL THEORY

For the purposes of this thesis non-democratic forms of government such as communism are to receive little comment or analysis, instead the aim shall be to seek what form of democracy is either most pure or of greatest value.

There exists strong theoretical precedent for sortition's integral role in democracies from both ancient and modern political thinkers alike. Of the Greeks: Plato, Aristotle, and Herodotus all comment that selection by lot is more democratic than elections. This belief can also be seen in the work of Baron de Montesquieu, who wrote in his *The Spirit of the Laws* that, "suffrage by lot is natural to democracy, as that by choice is to aristocracy". Then again, care must be taken to differentiate various definitions of aristocracy with its translation from Ancient Greek being 'rule by the best' – ironically it is easy to see how one might question whether hereditary aristocracy in the modern world in fact leads to such an outcome.

Sortition's inextricable link to democracy historically means we may often find objections to its validity within arguments against democracy in the work of Plato. Within the *Republic*, the character of Socrates argues that if statecraft is in fact a craft then it surely follows that a master craftsman, with greater intelligence and morality, is required to lead the state. Further, Plato wrote of the issues that pluralities of opinion often cause in democracies. Similarly to aristocracy though, one must take care to note that democracy is best translated from Ancient Greek as 'rule by the mob'. It is on the basis of these two premises that Plato argues that the state should be led by 'philosophers kings' who benevolently rule in the best interests of everyone.

A complication is to be found though in that it appears Plato might have changed his mind in later life. His last dialogue *Laws*, which intriguingly is the only of his undisputed works to not feature Socrates as a character, seems to present a less extreme argument. Whilst still maintaining that the best form of government is that which is described in the *Republic*, Plato goes on to posit that the second-best state is one in which the citizens play an active role in sharing the activities of politics in a mixture of a monarchy and democracy. This 'mixed constitution' would later be adopted to great effect by the Roman Republic, and its theory developed by the likes of Cicero. Within the work of Aristotle there is also mention of sortition in an analogous manner, suggesting that its use is best for assemblies and juries but not for high office. Within Book 4 of his *Politics* Aristotle states that, "the power of veto, but not that of positive enactment, should be vested in the masses."

Edmund Burke, the 18th century MP and philosopher, was even more critical of sortition than Plato's early work – in stark contrast the same cannot be said of Burke's views on democracy more broadly though because as will be described, Burke advocated an elitist form of representative democracy instead. It is because of the close relationship between sortition and democracy that, to be able to understand sortition within a 21st century UK perspective, an understanding of wider democratic theory is required. Hence it will be the subject of the next section.

2.2.1: TRADITIONAL DEMOCRATIC THOUGHT

Of all the definitions of democracy it is perhaps that delivered by Abraham Lincoln at Gettysburg that is most informative. A democracy must be, "of the people, by the people, and for the people". Arguably however the democracy present in the 21st century UK fails on at least two of these criteria; many argue that we have an elite political class that rule in the interests of large corporations rather than the general citizenry instead.

Such arguments are predicated on the belief that one can truly assess a democracy's worth at all against certain criteria. Broadly, political theory suggests two ways in which this assessment may occur. On the one hand, there is an instrumental approach whereby the outcomes of said democracy are assessed and if they are good so too is the political system. On the other, a democracy can be good in and of itself, if it has desirable qualities inherent within its methods such as equality, justice, or fairness.

Further, it must be understood as to what makes a democracy legitimate: why the government is justified in undertaking a specific course of action. One approach, stemming from Immanuel Kant, is that the decision must have been arrived at commonly through public reason. An alternative, as proposed by Jean-Jacques Rousseau, is that democratic participation is that which is responsible for legitimacy. However the two schools are not mutually exclusive, with theories regarding deliberative democracy combining elements of both. The form of sortition that is to be proposed by this paper would be best classified as a form of deliberative democracy and therefore an analysis of it is to follow.

Deliberative democracy entails the people both being allowed to participate in political discussion and then, through debate, arrive at a decision as to the best course of action. One attack that is made is that people are self-interested, and as such deliberative democracy might not lead to what is in the country's interests. Indeed this description of individual behaviour is standard in traditional economic theory, and so some see its applicability to politics as self-evident. Others such as John Stuart Mill and Rousseau believe that people can be motivated by concern for abstract concepts such as justice or 'the common good' – it is actually argued by both that the process of deliberative democracy in fact enhances the propensity for this to occur. Whether one believes humans are capable of altruism then is likely to impact their desired design of democratic institutions considerably.

One approach to democratic theory that is to be, in large part, rejected within this paper is elite theory. Modern elite theorists, such as Joseph Schumpeter and Anthony Downs, present a view of democracy that is solely instrumentalist with Schumpeter, in particular, rejecting any moral connotations to democracy. His definition of democracy is a simply a system whereby elites compete through elections for the right to rule; the sole role of the citizens is to ensure the smooth and peaceful circulation of these elites. Schumpeter, whose key work *Capitalism, Socialism, and Democracy* was released in 1942, believed the 'average citizen' to be incompetent and unequipped to lead. Indeed Schumpeter later justified this position using empirical studies from the 1950s and 60s showing high public ignorance to current affairs.

One might be tempted to think that this was of frustration to Schumpeter,



but far from it. He in fact argued that this apathy was highly desirable as it enabled the elites to do their job unimpeded. Schumpeter's alternative was a highly motivated population of people who knew very little and were likely to pursue irrational yet appealing aims. Schumpeter did though think the people justified in overthrowing a tyrannical government – even if that does raise questions as to how such an ignorant population would be aware of such a phenomenon.

In relation to this thesis it is easy to see that an elite theorist would take issue with sortition, and likely any form of governance by the masses. Schumpeter did though see value in deliberation, so long as it were conducted by elites and in secret. It is also regrettably true that if Schumpeter were still alive he would likely cite the examples of people demonstrating political ignorance on social media as evidence as to why they ought not to be allowed a role in politics.

All of the above is not to say though that some of his work, even if unintended, might strengthen the argument proposed in this paper. One of the descriptions of democracy Schumpeter gave was that voters in fact play no role in political decision-making, rather it is politicians, and importantly political and economic interests, that do. As shall be discussed in the following chapter, this is in large part why so many are perhaps disenfranchised with modern politics in the UK. Furthermore, there is also merit in Schumpeter's views regarding the implementation of policy. It shall later be argued that even if a 'common good' is arrived at, it may still be hard to determine the means to that end; as such an elite theorist approach to the implementation of policy, once determined by the people, may be of use.

Charles Louis de Secondat, Baron de Montesquieu cannot go without mention here either. Montesquieu fervently advocated that, "a democracy must educate its citizens to identify their interests with the interests of their country". When a democracy fails to do so he argued that people begin to advance their own private interests at the expense of others through acquiring political power over them. It would seem then that, if successful, this process of aligning personal and national interest would resolve the issue early discussed regarding whether citizens are capable of truly voting for 'the common good'. Additionally, it is also helpful to understand the other reason Montesquieu provided for why democracies might fail, known as 'the spirit of extreme equality'¹. This phenomenon occurs when a country's citizens become no longer content with civil equality, instead desiring total equality. In this sense, we can see in the work of Montesquieu the seeds that would later grow into revolutionary socialism.

Modern political theory must also be considered carefully, as if a chamber from sortition would exacerbate real-world political issues that have been identified within academia a significant blow to this thesis would be dealt. The first major issue surrounding modern democracies relates to an apparent lack of inherent equality, with Tom Christiano highlighting in his 2004 paper *The Authority of Democracy* that, "in order for people to be treated publicly as equals they must have an equal say in collective decision making". A connected point is that the small role which citizens play in decision making leads to them having little responsibility for the outcome. Secondly, one must consider what the consequences of mass participation might be; for instance it can be argued that if all have equal political power it shall be diluted to the extent of impotence or, more commonly, that mass participation is not possible as it leads to the relative neglect of other key tasks in society. It is from this contention that one must then attempt to strike the balance

as to what role the ordinary citizen should play, and then further as to whether they shall be capable of doing so. To theorise of the ideal democracy one must also ascertain how once the will of the people is found it is to be implemented.

Within economic theory there is a key concept called the 'principal-agent' problem. First appearing in Thomas Hobbes' *Leviathan* the concept states that where actions are taken by an agent on behalf of someone else, in a circumstance where the agent disagrees with the intentions, then the task is completed less efficiently. Hence it can be argued that if a bureaucracy purely serves to implement public policy it has not determined then it is likely to do so in a worse manner than if the policy was of its own devising. In Hobbes' words, "it follows that where the public and private interest are most closely united, there is the public most advanced." For the purpose of this thesis it will later be argued that as a result of this, the executive ought to still play a role in the generating of legislation and / or receive recognition for successful implementation of policy.

2.2.1.1: DIRECT DEMOCRACY

A brief discussion shall now take place regarding what has been traditionally seen as the purest yet perhaps least viable form of democracy: direct democracy. Put simply, direct democracy can be understood as a system whereby every citizen of a state has a vote on each and every issue; as can be immediately seen though there are obvious logistical considerations that make it quite unpractical for large states.

Perhaps the most adamant defender of this form of governance was the 18th century philosopher Jean-Jacques Rousseau. In his 1762 magnum opus *The Social Contract*, Rousseau puts forward his defence of democracy and a conception of what provides it with greater legitimacy. To Rousseau, the citizens of a state should meet regularly to discuss issues and enact laws that magistrates are to implement. Pivotal to his framework is the conception that the majority decision represents the 'general will' of a people that is distinct from what is in the individual interest of each citizen. If one sees this using John Rawls' metaphor of the 'veil of ignorance', this concept can be interpreted that each citizen should vote for what is in the interest of the people as a whole so that if they didn't know their social position they would be happy of the outcome regardless. There is indeed an initial appeal to Rousseau's ideas, but it is issues of practicality that bring down its ingenuity. For instance, in all but the very smallest states it is not feasible for the entire populous to assemble, and to do so for every law would have a huge opportunity cost on the functioning of society. Moreover, Rousseau argues that in larger states it is harder for there to be shared common ground between citizens. As such it is evidently clear that the 21st century United Kingdom is not best suited to direct democracy and hence we use an alternative form which shall be discussed in the next section.

However, there are aspects of Rousseau's work which we might wish to consider in order to improve the UK's current legislature. Most crucially for this thesis, Rousseau's conception of political legitimacy ought not to be ignored: Rousseau argued that without active participation of ordinary citizens in politics, the system as a whole is illegitimate. Secondly, a modern interpretation of Rousseau's conception of legitimacy, which adds strength to the argument presented later in this



paper, comes through an understanding of the Condorcet jury theorem. First highlighted in 1785 by the Marquis de Condorcet, the theorem states that if each voter is more likely to be correct than wrong, then a majority of all is also more likely to be correct than wrong. More interestingly however is the fact that the probability that a majority will vote for the correct outcome increases with the size of the body of voters. David Estlund in his 2008 work *Democratic Authority* has thus described Rousseau's conception of legitimacy as, "the correctness theory", given Rousseau's desire for the whole populous to assemble in order for the correct decision to be arrived at. Hence in Chapter 4 a discussion will need to be had regarding the balance between this phenomenon and logistical practicality in regard to the size of the parliamentary chamber from sortition proposed.

2.2.1.2: REPRESENTATIVE DEMOCRACY

Given the impracticalities associated with direct democracies, most countries have long adopted a form of governance known as representative democracy whereby the populous elects individuals to represent them in the political process on their behalf. There are multiple methods to facilitate this, such as constituency elections or proportional representation, yet of huge importance is the distinction made by 18th century MP and philosopher Edmund Burke regarding the role of the representative. Either they are to be a 'delegate' who directly voice the opinions of those they have been chosen to represent or they act autonomously as 'trustees' and decide what is in the best interests of their constituents on their behalf.

There are merits to both conceptions – delegation would seem a purer form of representation, yet trusteeship benefits from its representatives being better informed and equipped with the time and resources to carefully consider political decisions. It would seem though that a mixture of the two cannot be enacted within a single chamber authentically. Furthermore, an important additional form exists called descriptive representation which relates to how similar characteristically the group of representatives are to the group of electors; for instance whether there is a similar proportion of women. The American political scientist Jane Mansbridge has argued that this form of representation is required when marginalised groups distrust those not also experiencing said marginalisation. In Chapter 4 a further discussion on this issue will take place when the case shall be made for a tricameral parliament which would incorporate many of the benefits of each form whilst protecting against flaws too.

Intriguingly, in contrast to Jean-Jacques Rousseau in the previous section, some such as American founding father James Madison have argued on behalf of representative government not on grounds of practicality but rather that representatives are less likely to sacrifice the long-term prosperity of a country for short-term personal gain; an outcome which might be all too easy if every person had a vote on every issue. On the flip side, elected legislators might have more experience governing or competence at it, however they also tend to represent a smaller section of the population. This is compounded by the prevalence of single member district representation which often requires just a simple plurality for election victory, resulting in the suppression of minority opinion and interests. Consequently, it is this systemic underrepresentation of

minorities that leads Bernard Manin to suggest in his *The Principles of Representative Government* that representative democracies aren't truly representative at all. Moreover Charles Beitz forcefully argued in his 1989 work *Political Equality: An Essay in Democratic Theory* that single member district representation encourages moderation in policy designed to appeal to the median voter in order to gain the most votes. Whilst this might initially appear a good thing, it can also be seen to lead to excessive continuance of the status quo even when it is entirely in need of fixing.

One final theoretical interpretation of representative democracy that shall be discussed is that of John Stuart Mill. Like Burke, Mill was a strong defender of representative democracy although notably Mill didn't see the primary purpose of government representatives as the generation of legislation. Rather, in his eyes, parliaments are best suited to be places of debate on public opinion and further they should ensure that the executive is effectively administering the laws and policy that parliament has enacted. A summation of Mill's thoughts in his own words from *Of the Proper Functions of Representative Bodies* is as follows: "Their part is to indicate wants, to be an organ for popular demands, and a place of adverse discussion for all opinions relating to public matters, both great and small; and, along with this, to check by criticism, and eventually by withdrawing their support, those high public officers who really conduct the public business, or who appoint those by whom it is conducted." It is along these lines that a chamber from sortition shall later be argued for.

As has been seen, on practical rather than malicious grounds, representative democracies are designed to exclude citizen participation. If instead ordinary people can be placed at the heart of government we might truly one day have government of, by, and for the people. In order to achieve this, it shall be later argued, we need sortition not voting, even if there does exist a 21st century assumption that democracy logically entails elections.

2.3: CURRENT APPLICATIONS OF SORTITION

Regarding sortition's modern application it is to be observed that it plays a lesser role in modern political life. Indeed where it is used, as shall be outlined, it tends to be in order to decide upon specific issues as opposed to the creation of a body that will make many such decisions.

2.3.1: COMMON LAW JURIES

The United Kingdom has long utilised juries, selected randomly, for criminal cases with the argument for their use often that decisions relating to criminal cases are of such importance, for not only the individual being tried but society too, that they should not be left to a judge to determine. Instead, a verdict is returned by a twelve-person group of ordinary citizens and then a judge sentences or acquits accordingly. Since 1921 it has been the case that women have been eligible to be on a jury and so selection of jurors is now done randomly from the adult population as a whole. Other countries, ordinarily ex-colonies of the UK have adopted similar legal systems and so the process is repeated similarly throughout the common law world.



2.3.2: CITIZENS' ASSEMBLIES

Another modern use of sortition that is vital to be understood in respect to this thesis is the selection of citizens' assemblies. Citizens' assemblies are bodies of quasi-randomly selected citizens and they intend to provide a forum for discussion on an issue, and then a decision reflective of the educated public opinion. In order to fulfil this function, the members of the assembly are provided with access to experts on an issue before they discuss and deliberate the topic collaboratively as to what is the best outcome. For the sake of manageability, and to ensure fruitful deliberation, the selection of participants tends to be limited to between 50 and 200 people and their selection is carefully intended to reflect a cross-section of the wider population. As shall be discussed, the process of formation is not without flaws but broadly speaking most would agree that they are fairly representative. Further, an inherent benefit is that they allow for the representation of the common person whilst ensuring that ignorance to an issue is not a factor. Deliberation, it is also argued, removes factionalism by emphasising a pragmatic resolution as opposed to partisanship.

2.3.2.1: IN PRACTICE

To grasp how and why citizens' assemblies function a few examples will now be given to serve as illustrations. In 2006 and early 2007 two Canadian provinces, namely British Columbia and Ontario, organised citizens' assemblies to discuss electoral reform – the Netherlands conducted a similar process in 2006 too. In all three cases participants were chosen by a semi-random process that ensured both geographic and demographic diversity: invitations were sent out randomly to people on the electoral register and they were asked to either consent or decline to be considered as eligible. The selection process was then applied to those who opted in, and then those selected were informed.

In the case of British Columbia those selected received introductory courses in electoral politics for twelve weeks in what was dubbed the 'learning phase'. After this the participants entered a 'public consultation phase' where dozens of hearings were held and over 1500 written submissions were discussed. After which they deliberated among themselves before voting on different options in three separate votes.

One major flaw in the process used was that due to the voluntary nature of participation there was a disproportionate number of members of the assembly who held strong views on the topic. In British Columbia's assembly, for example, polls showed that whilst the wider public were satisfied with the electoral system, the majority of participants were strongly dissatisfied. Amy Lang, from the University of British Columbia's Centre for the Study of Democratic Institutions, however noted two distinct benefits of the body chosen. The vast majority of participants showed an interest in learning about the issue, and a commitment to the process which she argues, "is likely to have contributed to the excellent working dynamic within the Assembly"². Michael Pal was more critical of the outcome in Canada saying, "the requirement of an equal number of members from each electoral district resulted in Assemblies that did not reflect the actual population"³. As such, perhaps a lesson needs to be learnt regarding whether to prioritise demographic rather than geographic representation.

Citizens' assemblies have also been used in the Republic of Ireland recently, to perhaps surprising effect. Two assemblies, one in 2013,

and another in 2016, were formed to discuss and debate the morally contentious issues of gay marriage and abortion respectively. Following similar procedures to other examples, both assemblies voted in favour of legalisation. Any critics of legitimacy were then proven wrong when their decisions were subsequently approved in national referendums by 62% and 66% of votes respectively. Given the role that Roman Catholicism has traditionally played in Ireland both outcomes were large breaks from any perceived existing status quo of moral sentiment. There is a strong argument to be made that if even these highly contentious issues can be deliberated upon by citizens' assemblies, in a manner reflective of wider public opinion, then it is surely the case that 'ordinary' laws can be too. It will later be argued that any complaint of competing claims to legitimacy regarding legislation can be avoided by implementing citizens' assemblies into the existing UK parliamentary framework.

2.3.2.2: THEORETICAL IMPLICATIONS

Intriguingly polls showed that during and after the process in Canada the perception from the wider public was that the assembly members were both technical experts and ordinary citizens simultaneously; an arguably ideal scenario for legislators. Further there is much to be desired in the manner in which issues affecting politicians can be dealt with *not* by said politicians.

Citizens' assemblies also lead to discussions about deliberative forms of democracy more broadly. Many have argued that deliberative models of democracy, to a greater extent than others, lead to ideal levels of: impartiality, rationality, and knowledge of the facts. If one also accepts that an increase in these conditions leads to a greater probability of good decisions being made, then it follows that deliberative democracy has a value in producing good decisions.

A key question that does arise from the use of citizens' assemblies though is whether the assembly itself should be capable of choosing its own agenda or whether it should be pre-determined. As we have seen in the case of British Columbia, the participants had their agenda defined by the legislature rather than themselves. Many have stated, in agreement with Yale political scientist Robert Dahl that in an ideal democracy the ability to set the agenda must be vehemently protected. In Dahl's words, "the body of citizens ... should have the exclusive control to determine what matters are or are not to be decided"⁴.

Another, arguably the most important, ramification of how citizens' assemblies function is that, due to the random selection process, they allow for a diverse range of problem-solving methods and ways of seeing the world – a phenomenon henceforth referred to as cognitive diversity. Deliberation, it can be argued, is improved as a consequence. It is not hard to see that traditional politicians tend to have very similar environmental conditioning: they are almost all university educated for example. This narrowing of approach is recognised to be detrimental in all walks of life, with many companies admitting that it is their intention to hire graduates from a wide range of subjects for this very reason.

A common attack on citizens' assemblies is that they lack expertise, or in more elitist terms, they lack those people that have the skills to make political decisions: Schumpeter's argument follows a similar structure. If therefore it can be demonstrated that this lack of expertise is not to the



detriment of sortition-selected assemblies but even to their benefit there are obvious benefits for the integrity and validity of sortition. Lu Hong and Scott E. Page have perhaps done so: the pair conducted a study where it was found that a team of individuals selected from a diverse population of intelligence outperformed a team comprised of the most intelligent people of the population only.⁵ Furthermore, this argument has been developed in a political context by H el ene Landemore who argues that the random selection of representatives would result in greater efficacy, diversity, and inclusivity than elections.⁶ Indeed it should be noted that this argument is not entirely new either, with the 19th century MP and philosopher J.S. Mill stating that governing assemblies should be a "fair sample of every grade of intellect among people" rather than "a selection of the greatest political minds".⁷

2.4: PROPOSED AND ACTUAL POLITICAL IMPLEMENTATION OUTSIDE THE UK

This section shall outline other use cases that have been theorised for sortition whether they be relating to foreign legislatures or other ideological frameworks. Perhaps the simplest yet least descriptive application of sortition is that advocated by the French political activist  tienne Chouard who proposes replacing elections with sortition. Yet it would seem evident that a more complex implementation plan is likely to be required to both convince a sortition sceptic of its value and to ensure it could be implemented to good effect.

Perhaps the best starting point for a discussion of this nature would be with the Marxist political theorist C.L.R. James who wrote an essay in 1956 entitled *Every Cook Can Govern: A Study of Democracy in Ancient Greece, Its Meaning for Today*. Within it, James suggested that a large legislative body, such as the U.S.

Congress, could be selected through sortition from the adult population at large: arguably this work was responsible for reinvigorating academic interest in sortition. One development of this idea of James' has come from the anarcho-capitalist writer Terry Hulsey who proposed a 28th Amendment to the U.S. Constitution which would randomise the selection of every member of both chambers of Congress.⁸ A different advancement of James' proposition came from Ernest Callenbach and Michael Phillips in their book *A Citizen Legislature*. Callenbach and Phillips are less radical than Hulsey and suggest that only the House of Representatives should be replaced with sortition, and it should be done so on the basis of its provision of: fair representation for the people and their interests; a minimisation of realpolitik; and the removal of the influence of money – and any associated corruption. The combination of which, they argue, would lead to better legislation.

Similar types of application have been theorised regarding other countries too, with political science scholars from Copenhagen Business School positing a supplementation of the Danish parliament, the Folketing, with another chamber of 300 randomly selected Danish citizens in order to combat elitism and career politicians in a book entitled *T em Eliten*, or in English *Tame the Elite*. Furthermore, during the French presidential campaign of 2017, Jean-luc M elenchon proposed a sixth republic for France whereby the upper house of its legislature would be formed through national sortition. Yet perhaps the best European example, or at least the best realised, is that of the Parliament of the German-speaking Community of Belgium. A permanent Citizens'

Council, comprising 24 citizens randomly selected for an 18-month term, organises regular citizens' assemblies to discuss contentious political issues. Following the assemblies' verdicts, the German-speaking parliament is constitutionally required to discuss the recommendations made.

On a more abstract level, both the aforementioned Robert A. Dahl and Simon Threlkeld have presented a different take on the application of sortition. Dahl argued in his 1989 work *Democracy and Its Critics* that an advanced form of democracy could exist centring around *minipopuli*. Dahl argues that a group of ~1000 citizens selected randomly from the entire *demos* could either set an agenda of issues or deal with a particularly major one. These *minipopuli* would hold hearings; commission research; and debate and discuss. It should be noted that Dahl envisages them as supplementing rather than replacing legislative bodies. Threlkeld meanwhile proposes that laws are decided by legislative juries rather than by elected politicians or referenda.⁹ Existing legislatures would still exist, and could propose laws to the legislative juries, but could no longer pass laws. Threlkeld also notes that individual citizens, as well as public interest groups, would also be capable of proposing laws to these legislative juries.

Arguably the most complete theory proposed however is that presented by David Van Rebroeck in his *Against Elections*, designed by the political scientist and ex Vermont congressman Terill Bouricius. Bouricius was heavily influenced by classical Athens and suggests a system whereby there exists: an Agenda Council which chooses topics for legislation, thus addressing Dahl's complaint regarding agenda-setting; a Reviews Panel which develop legislation; and a Rules Council which can adjust the legislative process itself. The members of all three bodies are selected via sortition from volunteers for 3-year terms and are paid handsomely. That is not the full picture though, as Bouricius then proposes a Policy Jury, which holds the authority to vote bills into law. A new jury is assembled for each piece of legislation, and its 400 members are selected again through sortition, but this time from the entire adult population rather than volunteers: those selected are obliged to participate, much like a trial jury. The jurors only serve for a few days, during which time they receive objective information about the legislative decision in question and hear arguments for and against each of the options before voting in a secret ballot. The aim of Chapter 4 shall be to try and present a plan for implementation in the UK that describes the process to a similar degree of detail as Bouricius whilst also retaining the benefit of being through reform of existing political structures rather than reconstitution.

A last point of note is that whilst sortition was born out of, and should be directly linked to, democracy, some theorists have highlighted its applicability in a non-democratic sphere. Having been influenced by John Burnheim, the Marxist economists Allin Cottrell and Paul Cockshott have proposed that in a post-capitalist society sortition could be used to ensure that a new social elite would not form.¹⁰

2.5: RECENT IMPROVEMENTS FOR SORTITION

Since its first use, the manner by which sortition can be undertaken has changed dramatically. Furthermore, it has become easier for larger groups of people to be eligible and considered without complicating the process, as stratified sampling can now be used thus ensuring



greater perceived fairness. Additionally, modern research by Carnegie Mellon University has shown that sortition leads to outcomes that are likely representative of a wide range of groups and opinions.¹¹

Moreover, there is another piece of research applicable to this paper that is of great importance. In 2011, a study called *Accidental Politicians: How Randomly Selected Legislators Can Improve Parliament Efficiency* was published in a physics journal called *Physica*. The researchers from the University of Catania in Sicily found that when some legislators are selected randomly, with no party allegiance, the overall efficiency of the legislature improves with regard to both the number of laws passed and the average social welfare obtained from the new laws. Furthermore, the relatively recent phenomenon of extensive census and demographic data will be pivotal for the thesis presented in this paper.

CHAPTER 3: UK GOVERNMENT AND POLITICAL CLIMATE

“The people of England deceive themselves when they fancy they are free; they are so, in fact, only during the election of members of parliament: for, as soon as a new one is elected, they are again in chains, and are nothing. And thus, by the use they make of their brief moments of liberty, they deserve to lose it”

Jean-Jacques Rousseau's *The Social Contract* (Book III, Part 15)

3.1: BRANCHES OF GOVERNMENT

The United Kingdom is a liberal representative democracy and, as is typically the case, has three branches to its government: an executive, a legislative, and a judicial. It does not however have the inter-relationship between these branches, facilitated by checks and balances, that Montesquieu posited as ideal; in large part because it is a system that has been evolving far longer than Montesquieu's work has existed, let alone had influence. Consequently it is the case that there is a fusion of powers between the UK's executive and legislative branches with it being a constitutional convention that all ministers must be drawn from either House of Parliament. Moreover, a central tenet of the United Kingdom's unwritten constitution is that parliament is sovereign. The combination of these two points mean that the executive only remains in office so long as parliament has 'confidence' in it.

Historically speaking, as a result of the principle of parliamentary sovereignty, the judiciary has played a rather deferential role regarding political and /or moral questions, with it often having been the case that an issue will be decided to not be one for the courts but rather for parliament. Increasingly though that is changing, with Lord Sumption an ex Supreme Court judge, delivering the 2019 BBC Reith Lectures on the increased frequency with which the judiciary is being asked to resolve these contentions; even if that may be entirely undesired.

Sumption's line of argument within those lectures, and the book he subsequently penned, is that the UK is in a state of political turmoil where traditional practices and conventions are being increasingly ignored. The crux of his argument, that is applicable to this thesis, is that issues that are inherently controversial ought to be dealt with by a democratically accountable and representative body, in effect thus out ruling the courts. Yet, more and more, parliament is not dealing with these issues itself, instead choosing to defer to the courts. It is then

suggested that the reason for this phenomenon is that parliament is perhaps unrepresentative of the wider public, and so the legislature is unsure of its legitimacy in determining laws on such contentious issues. Sumption doesn't however provide a solution to the trend, with his focus a negatively defined one regarding what ought not to happen. The remainder of this paper will present a potential solution to the issue that is consistent with all other aspects of Sumption's reasoning.

3.2: PARLIAMENTARY SYSTEM

It has long been the case that the United Kingdom has had a bicameral legislature, with a House of Commons and a House of Lords; the former being elected, the latter not. Whilst historically speaking the Lords was the pre-eminent chamber of the two, within the last two centuries that has increasingly ceased to be the case. For example, it is now conventionally the case that the Prime Minister is drawn from the Commons rather than the Lords – this has not always been standard though, with more 19th century Prime Ministers being Lords than MPs.

The Parliament of the United Kingdom is best described, as first done so by Conservative peer and academic Baron Norton of Louth, as a policy-influencing rather than a policy-generating legislature, given that it is the executive that proposes bills. This is in contrast to the United States which has a greater degree of legislative independence. For a piece of legislation to enter UK law it must be passed in both houses before receiving the purely superficial Royal Assent. This split voting is, at least theoretically, to be desired as it provides a balancing of power and a check on potential tyranny, however in the last century or so this benefit has been of a lesser concern than it might have been traditionally. Whereas it used to be the case that both houses had to approve a bill, without exception, for it to become law, the Parliament Acts of 1911 and 1949 sought to change that on the basis of democratic legitimacy. The motive being that an unelected upper chamber should not be capable of blocking what is, theoretically at least, 'the will of the people'. The 1911 Act made it so that the Lords could block a bill for only two years after it had been passed in the Commons, and then the 1949 Act shortened the period to one. Consequently the balance of power shifted considerably towards the Commons.

3.2.1: HOUSE OF COMMONS

The House of Commons today is a democratic body that is elected using first-past-the-post on a supposedly five-year basis, as stipulated by the Fixed-term Parliaments Act of 2011. It consists of 650 members who each represent a geographic constituency of ~70,000 people.¹² Almost all MPs, the abbreviated term for members of the House of Commons, belong to political parties. A consequence of this is that MPs are under the control of their party with regard to policies and agenda; which tend also in turn to be controlled by other economic or political interests. The largest party in the house then ordinarily forms a government and becomes the executive.

In theory, the House of Commons is supposed to fulfil a number of non-legislative functions including: debate, representation, and scrutiny of the executive. Both the latter and legislation itself though are massively affected by party membership. All ministers are bound by the convention of collective ministerial responsibility which means that they cannot vote against the government; this is important as it means that their constituents' best interests are often not being represented. Further, MPs



are instructed by their parties as to how to vote on legislation which means that often they cannot vote with their conscience as to what path of action is actually best. Whereas the Commons is supposed to deliberate on what is in the country's best interest, it is often, as political scientist John Dryzek described Australia's federal parliament, "a theatre of expression where politicians from different sides talk past each other in mostly ritual performance". It is not a stretch to suggest that party politics crowds out true deliberation. A further point for discussion is how representative the House of Commons actually is. The politically active are over-represented given that the vast majority of ordinary citizens not affiliated to a party. Furthermore, the Commons is far from descriptively representative with only 34% of MPs women, while 51% of the population are female; there is a similar such issue with ethnic representation with 10% of MPs non-white and 14% of the population so.¹³

3.2.2: HOUSE OF LORDS

The House of Lords' function and membership have drastically changed in recent times. In the past only a member of the hereditary peerage or senior Anglican clergy were eligible for a seat whereas that has significantly changed. In 1958 the Life Peerages Act was introduced which initiated the now common process whereby a person is given a seat in the House of Lords and the associated title of Baron or Baroness but only for the period of their lifetime – it cannot be inherited by their children. As a result of this, over time the makeup of the House of Lords has shifted considerably with more and more people with backgrounds in public service entering the chamber and providing it with increased specialist expertise; a large number of which sit with no party association. Furthermore, those from finance and industry bring skills that are much needed for policy revision. By the 1990s almost half of the chamber consisted of these 'Life Peers' with the other half being the traditional hereditary peers. As shall be eluded to in the next section, this would dramatically change when New Labour came into office in 1997, following large public desire for reform. A last point to note is that some members of the House of Lords do indeed serve in the executive, some even in the cabinet, although this is uncommon.

3.2.2.1: RECENT REFORM

When Labour won the 1997 General Election many expected the House of Lords to be significantly reformed, and in some senses it was but just perhaps to a far lesser extent than was expected. The following section seeks to outline the actions that were taken by that government to reform an institution that many argued was undemocratic and outdated. A fair assessment can be made that suggests the focus was on the composition of the Lords rather than its relationship with the Commons. After entering government, Tony Blair appointed Lord Wakeham to lead a Royal Commission into House of Lords reform and a large number of proposals were submitted and then recommended. Many of those not acted upon shall be discussed in the following section, but the largest change made was to expel all but 92 hereditary peers from the Lords in order to reduce its then enormous size. Additional important changes were made to the role of Lord Chancellor but for the purposes of this thesis they are of little relevance.

During the Cameron-Clegg coalition there was further appetite for

reform, especially from the Liberal Democrat contingent, and Nick Clegg himself introduced the House of Lords Reform Bill 2012 which would have, amongst other changes, made the upper chamber mostly elected. Despite being issued a three-line whip, an effective compulsion, 91 Conservative MPs voted against the bill and it failed. Two years later however the House of Lords Reform Act would pass enabling Peers to retire, and to be removed from the House if convicted of a criminal offence and imprisoned for longer than a year.

3.2.2.2: NON-DEMARCHIC PROPOSALS FOR REFORM

The following section will outline many of the proposals for reform that were not adopted, so long as they did not advocate a replacement of the House of Lords with sortition. It should be understood that most opposition to proposals of sortition were predicated on belief in either the need for expertise or that democracy necessitates an elected upper chamber. A point of note though is that the 2007 Power Inquiry found that 68% of the public felt that the future of the House of Lords ought to be decided by a 'jury of the general public'; a method of facilitating such a state of affairs is precisely the purpose of this proposal. In contrast, only 17% responded that they felt it ought to be by elected politicians.

In broad terms almost all are critical of the current House of Lords, they just happen to differ in regard to why. The smallest and most radical group promote its removal, others suggest an entirely elected chamber, whilst some argue for the complete opposite in the form of an entirely appointed chamber. However, to further complicate, some suggest a mixture of the two, with no agreement then as to the proportion.

The simplest of reproaches against the Lords is that they lack diversity and thus representation, to a worse extent than the Commons even; and indeed statistically speaking they are right. As has been mentioned many, like Tony Benn, favour an elected house on the grounds it is more democratic. There are however difficulties regarding how this might be achieved without impacting the supremacy of the Commons.

Lord Steel meanwhile provided the best expression of the argument in favour of a fully appointed house in 2007 when he stated, "the great strength of the Lords is that it contains not just a bunch of experienced retired MPs but a whole raft of individuals with specialist knowledge and experience from the worlds of commerce, medicine, the services, the civil service, academia, the unions – the list is endless – none of whom would likely to be available to stand for election". All of the aforementioned groups, it would seem at least, add value to the chamber in a way the current 92 hereditary peers perhaps don't. Regarding a combination of election and appointment, it has been suggested that in doing so there would be a dichotomy between members, with potentially those who were elected suggesting they had greater legitimacy.

In summary, reform to the House of Lords appears to be a fine balancing act between a number of factors such as: how best to achieve a range of representation; the maintenance of specialist expertise; continuity of membership; the independence of the Lords; cost; and the potential clash between the legitimacy of members selected through different means.



3.3 POLITICAL PARTICIPATION

Political participation refers to the role that the citizens play within the political process and, with rising populations and relatively static government size within representative democracies, less and less people are actually directly involved with the functioning of the government. Instead, when we talk of political participation in the 21st century most commonly we are referencing the level of political engagement of the public in response to not only issues but processes too.

Developing technology undoubtedly impacts the methods by which people can engage with politics in a positive way regarding ease, but many have argued that the modern world is full of 'clicktivism' as opposed to true activism; the signing of a petition or the liking of a social media post, it has been argued, does not represent true engagement. Many have gone as far to suggest that the UK is experiencing a 'participation crisis', leading to decreasing democratic legitimacy. This section will assess the methods that are available to citizens of the UK *polis* in the 21st century and how, if at all, they are being utilised and by how many. Assessing the status quo inevitably leads to historical comparison and indeed the English word for idiot comes from the Ancient Greek for 'one who does not engage in political life'.

A study by the Hansard Society in 2019 is vital in providing an overall understanding of political satisfaction in the UK: 72% of those polled say that the system of governing needs 'quite a lot' or 'a great deal' of improvement, with 37% choosing the latter option.¹⁴ Furthermore, the poll found that Britons have more confidence in the military and judges than in politicians to act in the public interest. These statistics must be continually remembered throughout the discussion in the following two subsections.

3.3.1: ELECTIONS AND REFERENDUMS

Of all the methods to participate in a representative democracy the most obvious and direct ways are to vote in elections and referendums; closely related is party membership and so it shall be discussed too. Whilst electoral turnout has increased since the first election of the century in 2001, it has perhaps still not risen to an acceptable level. In 2001, following the landslide election of four years prior, only 59% of people voted; 18 years later the figure was 69%. Arguments made relating to the civil rights struggles for suffrage suggest that this lack of voting is to be a serious concern, and there is obvious merit in their justification. Indeed in terms of legitimacy, it is the case that the second Blair ministry of 2001-2005 achieved a mandate from only 27% of the population eligible to vote and then orchestrated one of the most politically contentious actions in modern history upon deciding to enter the Iraq war. Following that decision, 750,000 people marched in protest in London alone: the UK's biggest ever demonstration.¹⁵

The integrity of elections must also be considered with: money, lobbyists, and the media hugely deterministic on the outcome. The UK admittedly has had less of an issue with monetary influence than the U.S. but it is still the case that vast quantities must be spent for a party and /or individual to stand any chance of being elected to political office. In fact, turnout was higher in the 2016 EU Referendum at 72% than the election of the year before, which had been 66%. Further, the frequency

of referenda has increased significantly in recent times which some have suggested puts strain on the integrity of parliamentary sovereignty, even if they are theoretically 'advisory'. It is because of claims of competing legitimacy that this thesis shall argue a quasi-referendum system within the workings of parliament would not cause an issue for the democratic legitimacy and the sovereignty of parliament.

Further arguments regarding referenda can also be assessed with relevance to the proposal of a parliamentary chamber through sortition too. For example, some argue that referendums provide an opportunity for direct democracy, yet a fair response would be that the arguments favouring direct democracy, over representative forms, tend to be attacks on representative democracy rather than strengths of direct – as such they are also favourable to a chamber from sortition. Further, whilst it is an unknown, the argument that referendums check executive power is likely to be applicable too. Yet even stronger is the obvious applicability of the argument that referendums enhance the legitimacy of a decision to a chamber from sortition, given that 'real people' are being consulted. Moreover sortition, as will be argued in this thesis, can be introduced without undermining representative democracy's expertise either. There are also additional flaws with the nature of how governments choose the wording and timing of referenda that would be addressed, and so too would inaccurate assertions during campaigning be avoided. Of huge weight also is that the proposed system would attempt to avoid self-interested voting, instead promoting a Rousseau style 'common good'.

Regarding party membership, it was once seen as a cornerstone of political participation although in the last half century the figures have dramatically decreased. In the 1950s the Conservative party had a membership of 2.8 million people; the figure is now 180,000¹⁶. With less people participating in traditional political methods, for a complete assessment of the health of political participation in the UK we must now turn to less formal methods.

3.3.2: SOCIAL MOVEMENTS AND PRESSURE GROUPS

As previously eluded to, technology has provided opportunities for political participation not previously available such as: e-petitions, blogging, protesting on social media, and the organisation of protests online. In one sense it is hard to attack the opportunities that more people have to engage with politics, yet on the other it must not be to the detriment of other methods to have been a net improvement.

Both social movements and pressure groups have undoubtedly played increasingly larger parts in modern political life in the UK, with governments being incapable of just ignoring their arguments. In the last few years alone both Extinction Rebellion and Black Lives Matter have played a significant role in shaping the focus of both the media and politics. It is also the case that those advocating on behalf of both causes tend not to be those with great traditional political influence and so the popularity of both on social media has been integral to their furthering.

As such, it might be unfair to suggest that the citizens of the UK are politically disengaged but perhaps instead they are just disenfranchised with the current state of affairs. It has been seen that 72% say that the UK's system of governing needs 'quite a lot' or 'a great deal' of improvement, and perhaps sortition would go some way to enabling



issues such as these to be taken more seriously within the traditional political sphere.

CHAPTER 4: THE APPLICATION OF SORTITION TO THE UK PARLIAMENT

"Everyone who receives the protection of society owes a return for the benefit"

J.S. Mill's On Liberty (Chapter IV)

4.1: UNICAMERALISM

Within this chapter, a description of how a parliamentary chamber from sortition might work in the UK will be given on three different models. First will be a representation for if both current Houses of Parliament were replaced with a chamber from sortition, which is to be referred to as the House of The People. Secondly, there will be a description of how the House of Lords could be replaced with such a chamber whilst retaining the existing House of Commons; and then finally it shall be argued that the best scenario possible would be to reform both of the existing houses and implement the sortition-generated House of The People at the same time.

Unicameralism, the term used to refer to legislatures with only one chamber, is less common than bicameralism, or two-chamber legislatures, and is theoretically less desirable due to the lack of the effective check that a second chamber is supposed to provide. The following section seeks both to explain how The House of The People itself would function and why it would almost certainly function better in conjunction with another chamber.

Within a unicameral system, the House of The People would be free to set its own legislative agenda and to debate any issue it saw fit; moreover parliament as an institution would remain sovereign and any and all laws enacted by said house would be of equal standing to all existing UK statutes. As a randomly selected group of citizens, all well informed about an issue, motivated to find a good solution, and descriptively representative of the population, the house will come to embody the 'median voter' – as such its decisions will be seen in the same terms as Rousseau's 'general will'. The selection process would favour demographic rather than geographic diversity, with as best attempt as possible being conducted to ensure that the house is a microcosm of society at large. Compulsory voting would be used with the rationale that otherwise members are refusing to perform their function – much like how legal juries function. The house would have the right to call on expert witnesses, and much like a jury trial an impartial speaker would function as the judge to marshal the proceedings. Regarding how this person is to be selected, it should either be a member of the house who is elected by the other members; an appointed ex civil servant; or it is to be a role that the general public can vote for. Members would be expected to attend all sessions of the house – in that sense it would be a full-time job – and as such would be paid a commensurate salary with current MPs. There would also be expenses and an allowance for those unable to commute daily to stay in London during the week – an unfortunate necessary evil. Members, like trial jurors, are to be compelled to not be influenced by friends or family on an issue, and necessarily each member must be fluent in English and be a UK citizen. The term length would be one year, and

it would be seen as a civil duty to complete the term if selected; one wouldn't be capable of excusing themselves, as otherwise there would be a skew towards those most politically opinionated, unless of course it was on health grounds. The final procedural point to note is that once the chamber is selected algorithmically each year, there is to be a statement released highlighting the demographic accuracy figures whilst maintaining privacy of specific information about individual members.

There are many potential solutions to the question of how the will of the chamber would subsequently be executed; for example it could, in line with historical precedent, elect magistrates. Or, more likely, the current civil service would be retained, with the house monitoring its activity to ensure it is undertaking its policy implementation effectively. It is here where the idea of a unicameral parliament from sortition first falls down. As it stands, ministers have portfolios for which they are responsible and parliament can scrutinise their behaviour, yet under this system there would be no such executive accountability – this also raises broader points regarding the accountability of members of the House of The People too. Unlike the current system, the members would not be standing for re-election and thus there is no mechanism for the population to express its assessment on how each member is performing. Moreover, there is a contradiction in the idea that a deliberately autonomous member of the chamber should be subject to assessment in this manner in the first place. Unfortunately, this would lead to the only formal method of accountability for members of the executive being judicial review through the courts if wrongdoing was suspected.

A further contention that must be resolved is what size this chamber ought to be. As has been earlier discussed, direct democracy is not practical due to the numbers involved, yet the Condorcet jury theorem seems to suggest that the larger the body is the better. Indeed of note is a 2019 survey of UK citizens by the Royal Society for the Encouragement of Arts, Manufactures, and Commerce which found that 57% of people thought that a citizens' assembly would not be sufficiently democratic because it was not large enough.¹⁷ A proposed resolution would be that the house consisted of 1000 members, as this would be the largest size possible before its functioning would become impossible. Furthermore, as a multiple of 100, it would be easy to demonstrate percentages of representation effectively and simply to the population. Admittedly a house of this size would require compromise and effective procedures, but undoubtedly the benefits outweigh any negatives.

The last two issues that must be addressed in this section are how best to ensure that the whole population has faith in the house, hence leading to legitimacy; and also which factors ought to be prioritised over others in the process of achieving descriptive representation. The latter is an issue to which there is no easy answer, as one cannot easily ascertain which descriptors lead to which viewpoints and hence diversity of political opinion; a balance ought to be found between accurate representation of: age, education level, gender, religion, and sexual orientation though. To the first point, as was previously mentioned, there is a powerful conceptual connection in the modern world between democracy and elections and so it is likely many would be suspicious of sortition when implemented at all; let alone as a replacement for both existing parliamentary chambers. However this reticence to sortition as a concept entirely ought to be easily overcome once the case is made for sortition to the public: education is likely to



override instinctive fear.

The easiest benefit to convey is that under sortition, there would no longer exist those 'career politicians' which as Chapter 3 demonstrated are so distrusted. Closely related to this is that members of the House of The People would not be compelled by their party as to how to vote and are free from the reward-and-punishment system that operates in party politics – there would no longer be the warning to those unsure on an issue that if they don't tow the party line then they can expect little career progression. The role of political lobbying by economic and political interests would also be removed too. Simpler than either of those however is the basic argument from equality; sortition is truly egalitarian as all citizens have an equal chance of impacting law-making unlike the current system whereby ordinary citizens compete against those that have the backing of party support, and the resources that this support tends to bring.

Moreover, those that argue that sortition might be theoretically sound but don't believe it can be applied in practice need only look to the aforementioned citizens' assemblies in Ireland. In simple terms, a chamber from sortition would facilitate many of the benefits of direct democracy within a practically achievable framework that promotes equality and mass representation. Lastly, as we have seen, greater cognitive diversity – lesser intelligence and /or expertise included – leads to better outcomes than an approach focussed on bringing the best together. John Stuart Mill saw this phenomenon, in this exact context, nearly 200 years ago and yet some still make arguments that others are unfit to take part in political deliberation.

One can even argue that the implementation of sortition, and the potentiality of selection, is likely to lead to greater political engagement and self-education too. Regarding the classification of the type of representation that the house would bring, one can see evidently that near-perfect descriptive representation would be present, but more than that it is also true that, as a whole, the house acts as a delegate for the wider country; it is the mouthpiece for the amalgamation of all personal opinions that is popular opinion in the UK. It is from here that this thesis will attempt to polish the rough edges of sortition and propose how one might retain the benefits and dilute the downsides.

4.2: BICAMERALISM

Bicameralism is not only more common, being currently utilised in the United Kingdom, but it also has aforementioned theoretical benefits. As was eluded to in the previous chapter, many proposals were made to the Wakeham Commission arguing that the House of Lords ought to have been replaced with a chamber from sortition and it is to be remembered too that the likely reason for their lack of favour was the argument propounded by Tony Benn that democracy should logically entail a democratically elected second chamber. This section shall outline how the House of The People might function as a second chamber alongside a reformed House of Commons. Furthermore, a discussion will take place as to whether The House of The People would be capable of adequately fulfilling the role of the current House of Lords.

In simple terms, the suggestion in this thesis is that the current House of Commons would functionally remain the same, albeit it would change in name to the House of Representatives. As such, the executive would still be drawn from the House of Representatives, it too functioning in a

similar manner to how it does now. Further, the executive would still be responsible for the proposing of laws to parliament. It is clear that under such a system the de facto election of officials in the executive adds both democratic accountability and legitimacy. Moreover, this would also solve the principal/agent problem.

Whilst the role of the House of Representatives can be clearly conveyed, there is a degree of ambiguity regarding the best manner for the House of The People to function alongside it. On the one hand, it can, and has, been argued by some that a sortition-generated chamber would be capable of handling all of the existing functions of the House of Lords. Alternatively, there is some merit to the proposal of the House of The People acting as a convenient policy jury within the framework of the legislature. Both options will later be considered in turn, however before doing so a comment must be made on an intriguing proposition for how the House of The People could be generated in a bicameral system.

Michael Donovan in his 2012 work *Political Sortition for an Evolving World* suggests that the ratio of legislators elected versus selected through sortition should mirror voter turnout. Thus every individual who does not exercise their right to vote is in fact choosing sortition. For instance, if turnout was 60% then 3/5 of the parliament would be the House of Representatives whilst the remaining 2/5 would be members of the House of The People. In this way it is, in a certain sense, true that each and every election is also a referendum on electoral versus lottery representation. As interesting a proposal as Donovan has made, it shall not be adopted in this thesis on the grounds of simplicity and purity. Having round numbers of members is incredibly useful for voting purposes; and, in addition, for the relative size of both houses to be forever changing would take away a certain continuity that is to be desired. Instead, a similar selection process would be implemented as was outlined in the prior section. It is to be noted that fundamentally many of the benefits of sortition are unchanged in a bicameral application as in a unicameral one and so there will be little repetition regarding the benefits of sortition in and of itself, as the case for that has already been made clear.

Turning to the first of the two options, namely that the House of The People replaces the existing House of Lords, it would seem that there is an initial appeal. Many disagree with the partly appointed, partly hereditary, system that the House of Lords uses and perhaps sortition is the ideal replacement. The House of The People could consist of the same 1000 people, all lacking party affiliation, and they would also serve a one-year term, in line with the length of time the current Lords can block a bill from the Commons. However, on closer inspection, it becomes clear that perhaps the current function of the House of Lords is not best suited to sortition. As it stands, the vast majority of the work the Lords does is to scrutinise and revise policy, and to provide expertise – neither of which unfortunately sortition is suited for. Moreover, when it comes to scrutinising the actions of the executive, there too sortition is likely to be less efficacious given that the members selected are unlikely to have ever held public office themselves. Hence it would seem that this proposal is significantly flawed.

On the other hand the idea of the House of The People as a policy jury, by comparison, appears to result in a lesser number of issues. No longer would it be expected to actively edit policy, and no longer would specialist expertise be crucial. Rather the basic role of said house would be to agree or disagree with the intentions behind a bill, and



in doing so provide a view reflective of the population as a whole, if they were to have the requisite knowledge necessary to make such a decision. Perhaps the best way this could be implemented is through a two-stage advisory then veto process. When a bill is proposed by the government to parliament, in the first instance the House of The People provides an advisory opinion reflective of whether they agree with the intentions, which of course the executive could entirely ignore. However, once the bill has completed all stages of revision it is again put to the House of The People for a binding vote. If a simple majority vote in favour of the bill it passes, and if the reverse is true then it has been vetoed. Once again, the suggestion would be that members serve one-year terms and are incapable of abstention. By implementing this process within the existing legislative framework one also avoids claims of competing legitimacy, and it is for this reason too that the final decision of the house must be binding rather than advisory. This does, of course, require one to believe the house to be representative of the view of the wider public, however, as has been empirically shown, this is the case.

Regarding procedural detail, it is fair to say that significant change would be required to implement such a system. Members of the House of The People would need to be protected from direct lobbying, and the flow of information regarding a law would need to be managed and unbiased. One way of perhaps facilitating this would be an extension of the legally influenced process outlined in the previous section. Alongside the speaker of the house, whose job would be to martial proceedings, there would also be members of both the executive and opposition parties who would make their case for or against a bill. It is of crucial importance that opposition parties are allowed to voice their views, and for practical reasons every party with a member of the House of Representatives would be given the right to present. Perhaps there is also even some merit in there being a cabinet minister whose role is to oversee the proposal of policy to the House of The People, like lead counsel in a legal trial.

A further point for discussion is the correct role for lobbyists and social movements under such a system. Given that there would be an enshrined protection of members of the House of The People from lobbying it would only be prudent to outline an alternative. The easiest solution to this problem is to suggest that lobbyists make their case to the government and opposition parties who in turn promote their causes when addressing the House of The People. Unfortunately, such a system would only entrench many of the political practices that a chamber from sortition seeks to eradicate, such as the issue of insider political and economic interests having disproportionate influence on legislation. It would be all too easy for large corporates to lobby expensively given that their economic interests regarding an issue are great; meanwhile those with little influence might struggle to promote an issue that they care about just as intensely. Indeed unfortunately for this thesis, it would appear that there is no easy answer to this conundrum and as such it shall be left answered with instead an appeal to the net positives found elsewhere serving as justification.

Finally, a further hypothesis on the positive consequences of implementing sortition in this manner is that pointless bills are likely to be less common, hence increasing legislative efficiency. To see why this is relevant one need only think of a government with a large majority who is capable of passing a great many bills in an attempt to appear to be implementing new policy, whilst in fact all that is actually occurring is

a confusion of the body of statutes. Thus if an attempt can be made to limit legislation to cases with real justification it ought to be done so.

4.3: TRICAMERALISM

As a model for legislatures, tricameralism has far less historical and theoretical precedent than its lesser chamber counterparts. That is not to say it has never been implemented, however the best example is a rather unfortunate one. In 1983, apartheid South Africa introduced a new constitution which established a parliament with three chambers. The first chamber was called the House of Assembly and consisted of 178 only white members; the second was called the House of Representatives and composed 85 coloured, or mixed-race people; the final chamber, called the House of Delegates, was reserved for Indians with a membership of 45 members. Other examples include Simón Bolívar's model state and the three chambers of France's legislature during the Consular and then Napoleonic period. Many arguments are made against tricameralism, ordinarily on the grounds of its potentiality to be complicated, but the following section will seek to demonstrate why in fact the UK would be better off if it reformed its two existing chambers and introduced a new one.

Having it been demonstrated in the prior section that the House of The People would not be best equipped to fulfil the current role of the House of Lords, the case shall now be made as to why the House of Lords ought to be reformed into a new House of Appointees and at the same time a House of the People should also be introduced in a manner similar to that described in the previous section.

Under such a system the Commons would also change into the House of Representatives and the first-past-the-post voting system would be retained given that proportional representation, it will be shown, is achieved nonetheless in the form of the House of The People. Moreover, in terms of theorising the role that these representatives are to play, they are best described as simultaneously trustees and party representatives. In this sense they are likely to be bound by their party on many issues, and on free votes they are allowed to exercise their judgement autonomously in line with their outlook; thus indirectly reflecting the views of those that voted for them. In much the same manner as proportional representation becomes irrelevant in the House of Representatives, so too does the idea of requiring delegates.

Meanwhile, the House of Appointees would be composed entirely of appointed individuals, with the current hereditary Lords and the Lords Spiritual removed. The role of these appointees would be to act, independent of party affiliation, in the revision of policy proposed by the House of Representatives. This does though mean that no longer would members of the executive be drawn from the upper chamber. Further, once a member of the house is appointed they retain the role for life and are barred from standing for election again. Of note is that those who once held party affiliation are also eligible for consideration of appointment, although they do so on the proviso that they act autonomously from any future party guidance. In many senses this House of Appointees would retain the same constitutional role as the current House of Lords, however the issue of peerage must also be considered. On the one hand it can be argued that a life peerage is recognition of public service, yet on the other the House of Appointees ought to be seen as indistinct from the wider population, except on grounds of expertise. Perhaps a solution would be to replace the



existing life peerages with a similar system as is used for High Court judges where individuals are knighted, but do not receive a Barony and the associated title of 'Lord'. By doing so, these individuals retain a reward for public service without the contradiction that arises if one changes the name of the House of Lords to the House of Appointees without altering the nomenclature of the individuals that it is composed of.

Alongside the House of Representatives and House of Appointees there would be the introduction of the new chamber from sortition, also in this instance named the House of The People. Its role would be to supplement the current legislative procedure by acting as a policy jury in much the same manner as described in the previous section. At the point of policy proposal the house would vote in an advisory manner, and once both of the other houses had voted in favour of a law it would be voted on again in the House of The People which would have the power to veto. Given that, currently, a law having been passed in both the Commons and Lords then receives Royal Assent, it is to be proposed that this vote by the House of The People on whether to veto a bill ought to be called 'The People's Assent'. Beyond this stage, ideologically at least, it would be preferable if at that point a bill became an Act of Parliament, however if the current Royal Assent were continued this would have little meaningful effect on the symbolic power of The People's Assent. Another consideration to note is that the margin by which a bill passes in the House of The People would also be capable of being used as evidence to opposition parties of which issues they might wish to campaign on at the next general election. For instance if a bill passed with 90% in favour, then there is little ground to question its repeal, whereas if that number were closer to 55% the same would not be true. Once again, it is proposed that members of this house serve a term length of one-year, and it is also crucially again true that the House of The People would truly facilitate both descriptive and proportional representation within the legislature of the UK. Given that in this manner the benefits of sortition can be obtained, whilst also retaining the expertise necessary in an upper chamber, without an incredibly complex legislative process, it would seem obvious that if sortition is to be implemented in the UK, then it is in this manner it would best be achieved.

CHAPTER 5: CONCLUSION

"The best aren't forced to rule, so democracies get worthless politicians who pretend to be the people's friends"

Plato's Republic (Book VIII, 557)

5.1: FURTHER POTENTIAL ISSUES

It is understandable that any major political change is often met with reticence, and as such when proposing said change one should take care to address any concerns; not in the least because you wish all to be comfortable with the process of evolution or revolution, but also as it enables you to consider the potential weaknesses of your proposition and how you might attempt to rectify them. As such, the following section shall discuss some issues that might be encountered were a chamber from sortition to be implemented in the UK parliament.

First, a moral consideration regarding forced participation ought to be considered. In a liberal democracy citizens have, to a greater or lesser

extent, control over how to live their lives and, of course as such, the suggestion that an individual be forced to fulfil a role against their will is incomprehensible. However it is also true that in order for a House of The People to function effectively it must be truly descriptively and proportionally representative. Perhaps the best solution to this problem is to make participation a moral imperative – it should be seen as a civic duty in compensation for the benefits that society provides. This does though mean that individuals could, in theory, still opt out. Yet, much like jury service, there ought to be an associated stigma with doing so out of self-interest. Indeed hopefully being a member of a parliamentary chamber from sortition would be an enjoyable and rewarding role – even if not all sortition theorists would agree that this is ideal.¹⁸ It goes without saying that if individuals chosen decide to opt out then the process of selecting a replacement must find an individual who fits the right descriptive profile.

It is also evidently clear that the information presented to the House of The People would need to be impartial and objective. Clear standards must be followed, and all assertions justified – this is to avoid similar such situations as those we currently experience during referendums where inaccurate information affects the outcome significantly. One of the strengths of allowing opposition parties to present information is that interpretations by experts can differ, thus enriching the variety of advice presented. A related, but incredibly weak, argument against such a system is that this process of presentation would be both time-consuming and costly. However, in light of the severity of the task that the House of The People would be performing, such an argument would appear misplaced – if legislators don't deserve requisite resources then quite frankly who does? Moreover, another concern regarding time might be that the process of serving as a member of the House of The People is too time consuming to be practical – yet it is precisely because only 1000 individuals have to devote their working hours to the task that it is practical. Further, once again, any time expended as a member of the House of The People ought to be seen as time well spent fulfilling a civic duty to one's country. Closely related is that members of the House of The People would not have actively chosen to take on the associated workload of being a legislator, unlike their elected counterparts. This lack of will might then lead to less effective functioning of deliberation too. In response, the only reasonably defensible position to take, once again, is to ensure that the role of being a member of the House of The People is seen as one that should be undertaken in spite of personal hesitation.

Whilst it has already been highlighted, it is worth re-considering the lack of accountability of members of the House of The People. It is true that they would not be elected, but the same argument is also true of current members of the House of Lords. As has been seen though this in no way diminishes the importance of the role that the Lords currently play. The same would be true of members of the House of The People. Furthermore, when one considers that the only action the house can take is to veto rather than positively enact it becomes clear that the scope for tyranny is actually quite small. Lastly, one can also circumvent the problem entirely by suggesting that the members of the House of The People are the very people that they *are* to be held accountable to.

Integral to the entire argument for sortition presented in this thesis is that sortition, when implemented properly, leads to a microcosm of society as a whole. As such, even if it seems an obvious point to make, extreme care must be taken in the demographic stratification process to ensure



that the House of The People is truly representative of the population as a whole. As has been seen, this is far easier given modern technology, yet it cannot be forgotten that this process could quite easily be interfered with. Hence, the safeguarding of the computation process is of paramount importance.

Finally, an attempt to address some of the inherent problems associated with deliberation must be had. The two most pertinent are group polarisation, and the issue of how to deal with the contention between an apathetic majority and a passionate minority – in other terms, the balance between the number and the strength of preference. Cass Sunstein wrote in her 1999 work *The Law of Group Polarisation* that, “In a striking empirical regularity, deliberation tends to move groups, and the individuals who compose them, toward a more extreme point in the direction indicated by their own predeliberation judgments.” This issue can however be somewhat tempered by accurate briefing materials and unbiased expert testimony. Moreover, it is importantly also true that each member would be morally compelled to vote in ‘the common good’, not necessarily in line with their own personal views. Regarding the second issue, perhaps the best solution might be to make clear that the role of the legislator is not always to instigate policy but also to prevent unnecessary policy entering into law. Just because a few people are incredibly passionate about an issue it does not necessarily follow that to appease them is the best course of action; then again it might be, but this decision is still one that ought to receive the due care and attention it deserves.

It would seem then that sortition is not perfect, but then again is it ever really possible for a political system to achieve perfection? What must be considered, in truth, is whether on balance the case for a parliamentary chamber from sortition outweighs the potential downsides. It would also seem that there is a strong case to be made in support of sortition, and perhaps it is also true that many of the downsides discussed in this section are actually complaints that can just as easily be levied on existing UK political institutions. Ultimately though, as with anything, the decision regarding sortition is a personal one, and fundamentally it boils down to whether you agree with the analogy provided in the next, and last, section of this thesis.

5.2: A SYNTHESIS OF PLATO AND ROUSSEAU

Whilst the details regarding the implementation of an idea are incredibly important, they are perhaps less so than the reasons as to why something ought to be done. Many of history’s greatest achievements might never have happened were it not for the taking of a metaphorical leap-of-faith. It has in fact in many ways been shown that sortition is not new, and it can be applied in a manner consistent with existing principle and precedent. Those who wish to conserve tradition can find a lot in sortition’s application within a UK parliamentary chamber that is to be desired. Indeed the most important aspect of the United Kingdom’s constitution is the principle of parliamentary sovereignty, and here has been presented a way to increase the democratic legitimacy of the UK political system *without* infringing on that concept. Through sortition, the most pertinent issues regarding the functioning of democracy are given solutions. It combines the practicality of representative democracy with the greater legitimacy of direct democracy. Furthermore, it is arguable that as a consequence

of the lack of political party affiliation that would be present within the House of The People it would be better equipped to fulfil its vitally important legislative and deliberative functions.

The most effective way to summarise the thesis presented within this paper requires a return to classic political theory. As has been seen, Plato and Rousseau in many ways could not be more different. One advocated an, albeit supposedly benevolent and enlightened, absolute monarchy and the other fervently advocated on behalf of direct democracy stating that, “If there were a nation of Gods, it would govern itself democratically”. Rousseau then went on to say, “A government so perfect is not suited to men”, arguably due to the logistic complications of organising direct democracy – yet as has been demonstrated many of the benefits of direct democracy may be achieved through sortition without these complications. I shall now attempt to reconcile these apparently opposing thinkers.

Plato’s analogy of the ship of state argues that in the same way a ship should be led by an experienced captain, government should be led by an expert; he believed that the populous did not know how to, or indeed were not capable of, sailing the ship for themselves. In many ways, one must agree with Plato’s suggestion that expertise is vital – we cannot imagine being treated by an untrained doctor – yet his analogy of the ship of state is not entirely water-tight. Surely it is the case that the passengers on the ship, representative of the *demos*, ought to play a role in deciding the destination – the Rousseauian ‘general will’. As has been demonstrated throughout the course of this paper, in order to achieve this consensus of what is to be desired, a chamber from sortition is necessary. It is at that point, once the direction has been decided, that the captain’s skills, found in the executive composed of skilled elected members of the House of Representatives, are required – to guide the ship to the desired destination. In this way, we can indeed have the best of both worlds.



The Twelve Note Conspiracy: Exploring methods of comparison between various equal divisions of the octave

Stan Lawrence

INTRODUCTION

For the last few hundred years, Western music has mainly used a system called 12 tone equal temperament. This means it has 12 equally spaced tones before it reaches the same pitch as the first again, an octave up. This system is ingrained in our musical culture and isn't often questioned, at least in mainstream music.¹ However, some musicians maintain that there isn't any particular reason why this status quo should be continued. The microtonal composer Harry Partch even goes as far as to say that 12EDO (Equal Division of the Octave) is a "musical conspiracy."²

My aim in this project is to try and compare different EDOs. There are 12 semitones in an octave in the 12EDO system and there are 100 smaller divisions called cents in each semitone, so there are 1200 cents in an octave. Therefore, I need to divide 1200 by however many divisions I want in that octave then keep adding that amount to work out the number of cents in the different intervals in the chromatic scale. Here is an example of the simple arithmetic to work out 19EDO:

$$1200 \div 19 \approx 63$$

I have also shown which notes are closest to a Just Intonation major scale (specifically Ptolemaic, which is a tuning system connected to the naturally occurring harmonic series) - see highlighted in the table. I then entered all these numbers into a music producing program called Logic Pro X, which created a 19EDO chromatic scale.

As you can see in the far right column of the above table, the differences between Just Intonation pitches and certain intervals in the 19EDO chromatic scale are very small. This makes 19EDO quite a good **temperament**.

To explain what I mean by this, I will do so from the perspective from a 20th Century microtonal composer and theorist Harry Partch, who was strongly against the 12 tone equal temperament system. He posits his view in his landmark book *Genesis of a Music*.

The reason Harry Partch was so against the 12 tone system is because it is completely distinct from the intervals that exist naturally. When you half the length of a vibrating string, the note that it produces is exactly an octave higher than the original note. This ratio, 2/1, is the simplest ratio and therefore, Partch argues, the least dissonant³ (equal with

Interval	Number of cents	Closest 12EDO note	Difference from note	Difference from Just Intonation
1	0	C	0	+0
2	63	C#	-37	
3	126	C#	+26	
4	189	D	-11	-15
5	253	D#	-47	
6	316	D#	+16	
7	379	E	-21	-7
8	442	E	+42	
9	505	F	+5	+7
10	568	F#	-31	
11	632	F#	+32	
12	695	G	-5	-7
13	758	G#	-42	
14	821	G#	+21	
15	884	A	-16	+0
16	947	A	+47	
17	1011	A#	+11	
18	1074	B	-26	-14
19	1137	B	+37	
20 (+8ve)	1200	C	0	+0



the unison). In a concept that he calls Monophony, he says that the bigger the numbers in the ratio are, the more dissonant it is so that the fifth is made by the ratio $3/2$ so is also very consonant (but slightly more dissonant than the unison). Pythagorean tuning is a system which uses just those two very simple number ratios to build a whole scale⁴, which Partch would have agreed with to a certain extent. However, the problem of this is that there is sometimes a discrepancy when you stack intervals on top of each other that should get to the same tone. For instance, when you stack 12 perfect fifths on top of each other and compare that note with 7 octaves stacked on top of each other, there is a difference of 23 cents, which we call a comma.⁵

The Pythagorean system is a 3-limit tuning system which means it only uses ratios using numbers less than or equal to 3. If we use a 5-limit tuning Just Intonation system, we can use the slightly higher number ratios $4/3$ and $5/4$, for the perfect fourth and the major third respectively, which for Partch makes these intervals slightly more dissonant than the fifth or octave. 5-limit tuning still creates problems though and, again, we end up with a comma. Known as a systemic comma, equal to about 21 cents, this is created by the difference between stacking 4 perfect fifths and stacking 2 octaves with a major third.

So, in general, using Just Intonation creates problems and yet it is still considered the gold standard for tuning.⁶ Over many centuries, systems have been developed as a compromise which “temper out” the comma – and so these systems became known as temperaments. Today we mainly have Equal Temperament, which means that each semitone is equal. This may sound like a good thing but for Partch, it is a fundamentally flawed system, believing that “for some hundreds of years the truth of Just Intonation has been hidden... maliciously.”⁷ This is because all the intervals in this system (apart from the octave) are out of tune with Just Intonation, which is the system of purely tuned notes found in nature in the harmonic series. To squeeze each semitone into being exactly 100 cents, some very complex ratios must be used; for example, a fifth in 12TET is $2.996614/2$ instead of $3/2$. As Partch argues that the lower the number in the ratio are, the more pleasing they are to the ear, the massive ratios that have been worked out to make ET are dissonant. He explains this further by saying that the ear has to *jump* to hear the implied frequencies in ET, and that it wouldn't have to *jump* if the intervals were purely consonant like in Just Intonation. (See what Partch's solution to this was and criticisms of Partch in Appendix 2.)

One way to make a temperament is to use an EDO (though this is far from the only way). One can select certain notes from an EDO that are close to the Just Intonation or Ptolemaic equivalent and use them to create a scale, avoiding the problem of the comma. So here is 19EDO used as a temperament, followed by the 12EDO diatonic scale that we are so familiar with. It is subtly different to 12EDO and I like that sound.

However, I do not think that working out how close an EDO is to Just Intonation is a good way of comparing different EDOs. This is because my aim (even though that would be a completely valid and useful aim) isn't simply to create a temperament. To compare EDOs to Just Intonation assumes sovereign importance of JI.⁸ Surely just because it is found in nature this doesn't necessarily mean it has to sound better than anything else?⁹ And indeed, lots of EDOs are far off from Just Intonation and composers use these because of this as it is exciting to get new, unknown and other-worldly sounds (known as *xenharmony*).

This means that in order to compare EDOs, one needs a new framework. One could look at the characteristics or properties of a certain EDO and see how that makes it a useful, interesting or piercing sound. For example, 19 is a prime number so whatever interval you choose, if you keep going up by that interval, you have to go through every note before you get to the note you started with.¹⁰ If you stack minor or major thirds in 19EDO, you effectively get massive “diminished” or “augmented” chords spanning multiple octaves. This is different to 12-tone systems as 3 stacked major thirds or 4 stacked minor thirds gets you back to the original note an octave up but fourths or fifths you need to go through all the notes before you get to the original note (all these examples in Appendix 1). These kinds of simple mathematical properties differentiate between and enable us to compare EDOs and may make them appealing or not to composers.

However, I believe that the best way to compare EDOs is a more qualitative approach.¹¹ This is because the main reason people look at different EDOs in the first place is because they provide a completely different flavour to anything we have heard before, so we should take that as a starting point instead.

I learnt a lot from Partch's *Genesis of a Music* as he categorised the intervals of his Genesis Scale, putting the sound and purpose of the notes at the highest importance. This qualitative approach helped me understand that the most important thing is that the music I make sounds good to me. Music is an art, so it can never be the theory that is of the utmost importance. Inspired by this, I had an idea about comparing different EDOs by arranging versions of the same piece in each of the different systems. However, after I had completed this, I realised that what I had done was just to transpose a diatonic piece written for a 12-tone system. I had chosen the intervals that were closest in pitch to the 12 tone equivalent (although there was some artistic choice in some of the smaller EDOs as some of the intervals were pretty equidistant from the nearest 12 tone equivalent), which meant all I had done was created an out of tune major scale, from which I built chords and the melody. This did sound nicely out of tune and quite arresting for someone like me who had been surrounded by 12EDO my whole life. However, I felt that I hadn't used these EDOs to their full potential as I missed out a lot of notes and therefore harmonic colour and interesting tonal possibilities. But I still wanted to be able to directly compare the different EDOs (which included the original 12 tone system).

I came up with a compromise – to do variations on the melody and harmony (including on the original 12EDO version to make it a fair comparison) which used as many notes of that system's chromatic scale as possible.

THE PROCESS

My aim, as I said earlier, was to arrange a few different variations on one piece in different EDOs. I decided on *Mozart's Piano Sonata no. 16*¹² because it is instantly recognisable, has both conjunct and arpeggiated passages and it is completely tonal and diatonic. I only used the first eight or so bars because after that it becomes more chromatic, so wouldn't be possible on the simplest system, 7EDO. My compromise to make a comparison as fair as possible between the different systems was to arrange a variation using all of the notes in that system (but some of them I could only find a place to put them once or twice and a Weberian serialist technique where all the notes are

played the same amount of times would obscure the original Mozart Sonata completely). I also provided a chromatic scale of each EDO to accustom the listener's ear to that system, although it would probably take further listening to that EDO to become fully comfortable.¹³ I also arranged a 12-tone variation of the Mozart Sonata as a reference point. This wasn't just the same as the original – I added ornamentation to use all the chromatic notes in just the same way as the other EDOs.

7EDO

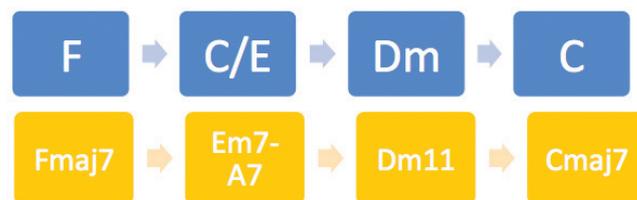
I started with 7EDO as it has the exact same number of different notes as the C major scale. This means that after I worked out all the exact number of pitches in the chromatic scale of 7EDO, I could program in the pitches in the same way as the original version. Obviously, it sounds vastly different to the 12EDO version as all the notes are spaced equally across the octave instead of both semitone and tone intervals in the 12EDO system. Five notes of the 7EDO mode is an approximation for a pentatonic scale found in Thailand¹⁴, so it is an ancient scale (although studies like these have sometimes been discredited as the tuning varies massively even between individual instruments). However, because 7EDO has so few notes, it is quite limited, so the harmonic palette is restricted.



19EDO

This system, used in Easley Blackwood's majestic *Fanfare in 19-Note Equal Tuning*¹⁵, took more thought as it was the first one I did where I had to make a "variation" on the original Mozart Sonata. I started by working out which intervals of 19EDO were closest in pitch to their Just Intonation equivalent and then made a 7 note "major" scale to be the main notes to base the sonata variation around. I then added ornamentation and passing notes to cover some of the other notes. Significantly, I also reharmonized the Sonata, partially inspired by listening to Sevish's otherworldly, jazz inspired 19EDO harmony in his EDM composition *What Year is This*.¹⁶ (I also replicated this same reharmonization on 23EDO and 12EDO, although it was impossible in 7EDO.)

From bars 4 to 8 in the original Mozart, the harmony descends with each chord being played twice (on beat 1 and beat 4). However, I decided that I would be able to use more notes of the EDO by changing the second of the repeated chord to a very slightly lower version of that same chord. As I had choices which notes to make up each chord – for instance having two options in the A in the Fmaj7 so making the A in the second chord the slightly lower version. I think that this makes the progression slightly smoother and this extra chord has a similar function to the simple tritone substitution in jazz music.



Original harmony (top) and my reharmonization (bottom)

23EDO

As 23EDO is one away from 24EDO, which is exactly twice the number of notes in the usual 12 tone system which makes it a simple quartertone scale, you might expect 23EDO to be quite similar and as wild as 24EDO or 12EDO. However, the unnoticeable difference of 2.17 cents between the interval size of each one stacks up pretty quickly. So much so, in fact, that it is the biggest EDO that does not act as a very good temperament at all, not having the vital 3rd, 5th and 7th intervals within 20 cents of the just intonation equivalent. This gives it quite an otherworldly and unusual sound and it is quite appealing to me. I also did a similar microtonal tritone substitution effect to 19EDO.



CONCLUSIONS

I really enjoyed and making these little arrangements. I find the harmony in these different EDOs so fascinating and it is inspiring to know that there are unlimited EDOs to try out, each with very slightly different harmonic colour.

However, I also think that, while it is near impossible to compare the EDOs quantitatively, it is also not easy to compare them qualitatively. My natural, impulsive description of each of the EDOs (other than 12) was that they were all alien, indescribable and chillingly, piercingly out of tune.

I was stuck between a rock and a hard place when I wanted to compare the EDOs. This was because when I made an arrangement, I couldn't simply have used the notes closest to Just Intonation or Equal Temperament as while this would have made a more easily comparable experiment, this would just be an "out of tune" arrangement of the original and also wouldn't use all the notes in that EDO. I did not set out to create a temperament to form an alternative to Equal Temperament or one of the many other systems that temper out the comma. So, I came up with a compromise: to make a variation of a piece, which would include all the notes in that EDO. However, this meant that each variation must be different as there are varying numbers of tones to fit in in each of the 4 EDOs I arranged. This, as I have found out, makes it hard to compare them.

It is also worth noting that, as society is entrenched within the "musical conspiracy" of 12-tone systems, it is extremely hard to break out of the 12-tone bias and compare other systems objectively. I agree with Joel Mandelbaum when he says that 12-tone systems will likely never be replaced on a popular scale. However, he goes on to say that "on an experimental scale [different EDOs] can co-exist with 12-tone."¹⁷

Furthermore, when I arranged the Mozart Sonata in different EDOs, I was in effect squeezing a 12-tone piece with 12-tone harmony into a non 12-tone system. Other EDOs can sometimes accommodate 12-tone harmony; however, this may also not be using these EDOs to their full extent – and having new harmonies is arguably one of the biggest advantages of new systems.

So, I created an original 19EDO composition called Stars in the Sea, which includes harmony that would be impossible in 12-tone systems. But as I was composing this, I realised I couldn't use any normative harmonic theory to develop chords to create a satisfying sequence. This meant it was a very slow process as I had to work out what chord I wanted from scratch. However, this is also what makes it all so overwhelmingly inspiring – the possibilities of different EDOs are almost endless.

APPENDIX 1

EXTRA RECORDINGS

12EDO circle of fifths

12EDO circle of fourths

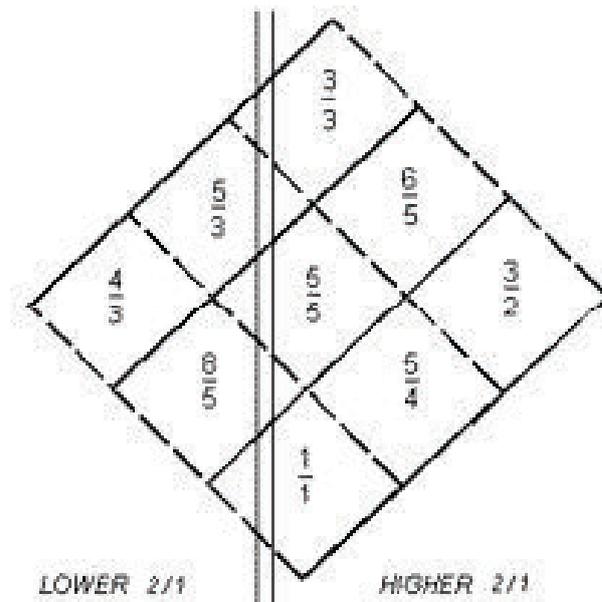
19EDO circle of minor thirds/diminished

19EDO circle of major thirds/augmented

APPENDIX 2

HARRY PARTCH'S SYSTEM

Partch invented his own system. He used something called a tonality diamond, an invention in which one can work out all the possible ratios from a given frequency. This is a 5-limit diamond, in which he only uses ratios built up from a fundamental starting point made of prime numbers less than or equal to 5. This makes it a very pure, Just Intonation system and so, according to Partch, much less dissonant than 12EDO. He wasn't satisfied with this, however, so he made an 11-limit tonality



5-limit diamond

diamond. He then added some extra notes so that all the intervals were roughly the same size and he was left with a monstrous 43-notes-in-an-octave scale which has been called the *Genesis Scale*. It is not an EDO because the intervals are different sizes, which means that it is like a tree in that it starts in one place and branches out, which means it cannot modulate and sound the same in another key.

Significantly, Partch divides all the notes in this scale into 4 categories: The intervals of Power, which are equivalent to our 4ths, 5ths and 8ves; the intervals of Suspense, which are our tritones; the interval of Approach, which are our 2nds and 7ths; and the intervals of Emotion, which are our 3rds and 6ths.

Petter Ekman critiques Partch in his thesis *The Intonation Systems of Harry Partch*.¹⁸ He describes Partch's methods as "unscientific" and having "inconsistencies" as Partch groups his different intervals arbitrarily and, significantly, without much notice given to the size of the numbers in the ratios of which he gave so much importance to before. Ekman says that in Partch's work we "hear the voice of the artist and the musician Partch and not the scientist." However, Ekman doesn't necessarily postulate this as a criticism as he says that "it may have been this inconsistency that resulted in his unique and beautiful music." Partch was guided by his ears and even if his ideas about Monophony and smaller ratios making more consonant sounds are wrong (Ekman posits that consonance may be completely subjective and Mandelbaum says that "the Cologne school and other groups hold that no small-number ratio possesses any special intrinsic value"), it doesn't really matter. At heart, Partch was a musician and he wanted to make music that sounded good. Levy agrees here that music is "above all, a matter of spirit and not of acoustics in the engineer's sense. Music... is not primarily something that happens in the air."¹⁹



Seeing the ups when faced with downs: the complex genetic phenomenon of Down's syndrome and its impact in our society

Theo Lakin

INTRODUCTION

In 2001, Karen Gaffney completed a relay swim of the English Channel. Six years later she swam the nine-mile span of Lake Tahoe.

Pablo Pineda, a Spanish actor completed his university degree in 2004 and went on to receive the Concha de Plata Award at the 2009 San Sebastián International Film Festival. He now works as a teacher.

Australian supermodel Madeline Stuart has appeared at New York, London and Paris fashion week and been featured in Vogue and Cosmopolitan after losing 20 kilograms weight to achieve her dream.

What do these three extraordinary people have in common? Namely a genetic condition called Down's syndrome.

Before the 1980s people with Down's syndrome were put into institutions, without adequate attention, education or medical care. They were neglected and essentially shunned from society for being 'no good'. A quote from a leading academic, American professor Joseph Fletcher in the 1960s; *"People [...] have no reason to feel guilty about putting a Down's syndrome baby away, whether it's "put away" in the sense of hidden in a sanatorium or in a more responsible lethal sense. It is sad; yes. Dreadful. But it carries no guilt. True guilt arises only from an offence against a person, and a Down's is not a person."* [FLETCHER 68]. This rather shocking statement was nothing strange at the time, but it just demonstrates the change in view of our society since then. I found this quote referenced in the book 'Far from the Tree' by Andrew Solomon. He uses this quote to highlight the view people had on those with Down's syndrome in history. Throughout his book he discusses what it means to bring up a child with a disability and offers a new perspective on life. Since 1983, the life expectancy for people with DS has increased by 35 years, from 25 to 60. Currently the oldest person alive with Down's syndrome in the UK is Georgie Wildgust, who turned 77 last year. Since the turn into the 21st century more and more people with Down's syndrome attend mainstream schools, more have graduated from high schools in the United States and more are going on to higher education. This change is recent, because of support and ambition, which has come about through a change in attitude.

It really has not been all that long for this large social change to have been made, and it just shows that once people see the reality, they stop focusing on what they consider perfection and learn to accept, support and enjoy. I am going to investigate the various aspects of Down's syndrome, looking into not only the genetics but also looking at its influence on life, for that of the person with Down's syndrome and those around them. I hope to offer historical, biological and social

understanding complete with some personal views and prospective. I want to understand why and show that despite the limitations of Down's syndrome, people with the condition can lead semi-independent, fulfilled and happy lives, all whilst improving society as a whole, by giving valuable lessons to those around them.

WHAT IS DOWN'S SYNDROME?

Down's Syndrome (DS) is a genetic condition which entails a set of physical, mental, and functional abnormalities as a result of an extra copy of chromosome 21 in the human genome, making 3 instead of the usual pair of two. This occurs during the creation of human sex cells (gametes) through meiotic division. It is a phenomenon known as trisomy 21, and it occurs in around 1 in 1,000 live births worldwide [THOMAS, 2019].

Down's Syndrome was officially recognised, and its characteristics described by John Langdon Down in 1866. However, it was not until 1958, some 92 years later that paediatrician and geneticist Jérôme Lejeune was able to find a genetic explanation for the condition. During a study of chromosomes of a child, he discovered the existence of an extra chromosome on the 21st pair. This was a significant milestone in genetics, as it was the first time in history a link was established between a mental disability and a chromosomal anomaly. Up until this point the condition was largely known as 'mongolism', after Langdon Down thought that cases of DS were a spontaneous step back in evolution from the supposed superior Caucasian race to the inferior Oriental race. This idea is absurd to us now, as well as extremely racist, and altogether a false representation of DS. The condition became known as trisomy 21, and increasingly over time called Down's Syndrome.

Since Lejeune's discovery, it has been shown that the characteristics and traits of DS are related to a small part of the long arm of chromosome 21, (21q22.1-21q22.3). This means the genetic material causing the effects is found between the first and third parts of the 22nd segment of chromosome 21. This small sub-section accounts for around 50-100 genes, which is a very small proportion of the whole human genome of around 30,000 genes [NEWTON, 2004]. All the genes of a human are contained within chromosomes, of which each person has 23 pairs in each cell, making 46 chromosomes. A person with DS will have 47.

Scientific research has shown that there are genetically three ways DS can occur with regards to chromosomal change. It is not a condition that is inherited, it is merely down to a chance error in cell division and can be diagnosed via blood tests. There are two different types



of cell division within the body, mitosis and meiosis. Mitosis is used for most of the body's needs, whether it be replacing old and worn out cells, or adding new cells during growth and development. It results in two daughter cells which are genetically identical to the mother cell and contains the same number of chromosomes (46), making them diploid cells. Meiosis, however, is a type of bodily cell division which has only one purpose which is to produce sex cells, known as gametes. The male gamete is a sperm and the female, an egg. It results in four daughter cells, as opposed to the two in mitosis. These four daughter cells display genetic variation and have half the number of chromosomes as the mother cell (23), making them haploid cells. This means that when the male and female gametes fuse during fertilisation, a zygote with the usual 46 chromosomes is created, a diploid. Meiosis happens in two parts, meiosis I and meiosis II. Genetic variation during meiosis is brought about by crossing over and independent assortment of homologous pairs during the metaphase of meiosis I.

The most common way DS is caused is called non-disjunction or complete trisomy 21, and it occurs during the formation of either a sperm or an egg in meiosis. The extra chromosome usually comes from the mother, and in less than 5% of cases of non-disjunction does it come from the father. Non-disjunction is the failure of homologous chromosomes to separate properly during meiosis. If a cell divides and it results in more chromosomal material going to one pole than the other, then the daughter cells produced will have an abnormal number of chromosomes. In the case of trisomy 21, when the cell divides, both chromosomes of the homologous pair are brought to one pole in a failure to separate, rather than one to each. This means that one of the daughter gametes produced will have 24 chromosomes, with two copies of chromosome 21. The other will of course have 22 chromosomes, and no copies of chromosome 21. When the gamete with 24 chromosomes, whether it be a sperm or an egg fuses with its opposite-sex counterpart, a zygote with 47 overall chromosomes will be created, 24 from the abnormal gamete, and 23 from the other. A usual zygote will have two copies of each chromosome, however in trisomy 21 there is an extra copy of chromosome 21. When the zygote divides by mitosis and the rest of the body's cells are created, they too will display this extra chromosome.

Another cause of DS is translocation. It accounts for between 3-4% of all cases of DS. Translocation occurs during meiosis when a chromosome breaks off and attaches to another chromosome. This means that during the metaphase of meiosis I, an extra chromosome is brought to one pole instead of the other, connected to one of the other 23 chromosomes. The chromosome which causes the features of DS is

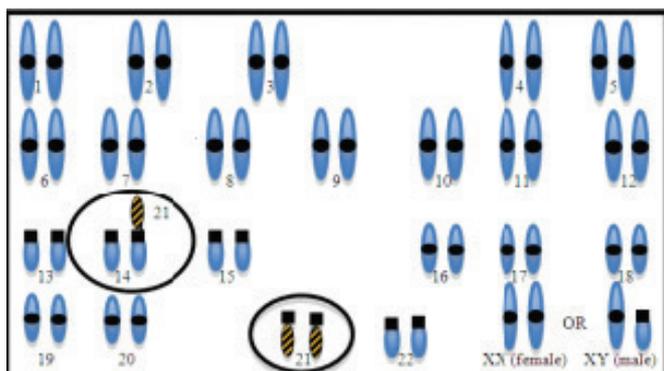


Figure 1 - a diagram of the human genome with translocation of the 21st chromosome, attached to chromosome 14

again the 21st which can be attached to chromosomes 13, 14, 15, 22, or in fact another chromosome 21. Few studies have been done to investigate the differences between those with translocation DS and non-disjunction, but they indicate that the differences are marginal, and they share essentially the same features [PRASHER, 1995]. The findings of certain studies, although requiring repetition with larger sample sizes do highlight an important area of further research. It is also possible, depending on how the chromosomes segregate on the equator of the spindle during meiosis, for the translocated material to go to the side from which it broke off attached to one of those 22 chromosomes. This is called balanced translocation, and the person will not display features of DS, as the correct amount of genetic information is present in the cell.

The third, and least common cause of DS is mosaicism. Mosaicism is a biological term which describes those who have two or more genetically different sets of cells in their body, meaning the chromosomal number within cells varies. While the other two causes were from errors during meiosis, mosaicism is from an error in mitotic cell division. As explained earlier mitosis is the body's main way for cells to divide, producing two diploid daughter cells that contain the same amount of genetic information as the parent cell. When an error occurs in mitosis the cell does not divide evenly into two. The result is that some cells contain 46 chromosomes, the normal 23 pairs, while others contain 47 or 45. The cells that then divide from the abnormal ones will also have that number of chromosomes. In the cases that cause DS, some cells will display trisomy 21 while others are normal. It occurs in one of two ways: either the zygote at first has three 21st chromosomes, which normally would result in simple trisomy 21, but during the course of cell division one or more cell lines loses one of the 21st chromosomes in a mitotic division error. The other way is vice versa; the initial zygote has two 21st chromosomes, but during the course of cell division one of the 21st chromosomes is duplicated. People with mosaic DS might have fewer characteristics of the condition than those with non-disjunction or translocation, if many at all; there is a variation. There has not been extensive research done to compare the two, however there was a report published in 1991 by K Fishler and R Koch which talked about mental development in Down syndrome mosaicism. It compared 30 children with mosaic Down syndrome with 30 children with typical trisomy 21. After IQ tests, it was shown that the mean IQ of the mosaic group was 12 points higher than the mean of the non-mosaic group. Despite this, some children with typical Down syndrome did score higher on the IQ tests than some of the children with mosaic Down syndrome, highlighting the variation. There has been an ongoing study project by the Department of Human Genetics at the Medical College of Virginia on children with mosaic DS. In a survey of 45 children with mosaicism, they found that these children did show delayed development compared to their siblings. 28 of these children with mosaicism DS were matched up with 28 children with typical DS for age and gender, and the children with mosaicism reached certain motor milestones earlier than children with typical DS, such as crawling and walking. However, speech development was equally delayed in both groups. It is certainly difficult to draw generalisations when the abilities of people with DS is so varied, but opens up possibility for further investigation.

DS is not a condition that is inherited, unless one of the parents of those with translocation DS themselves had a balanced translocation. In this

case the parent is said to be a carrier of translocation DS and display no characteristics, however the translocation gene can be passed on to the child. Other than this genetic factor, the only other real factor that increases the risk of having a child with DS is advancing maternal age. Older mothers have a higher individual chance of having a baby with Down syndrome. At age 45, the risk of a having a child with Down syndrome increases to 1/30. [NEWBURGER, 2000]. Research has been done to investigate the reasons for this, through studies involving mice. There are proteins present within cells that help keep chromosomes together at their centers. Lower levels of these proteins – called cohesin and securin – cause the chromosome pairs to be more loosely connected and further apart. In a study by Nabti, Ibtissem et. al, it was found that older female mice had lower amounts of these proteins in their eggs, suggesting that as the eggs age, the levels of these proteins fall. This can then be related to human mothers, implying that the causes of DS previously described are more likely to occur as a result.

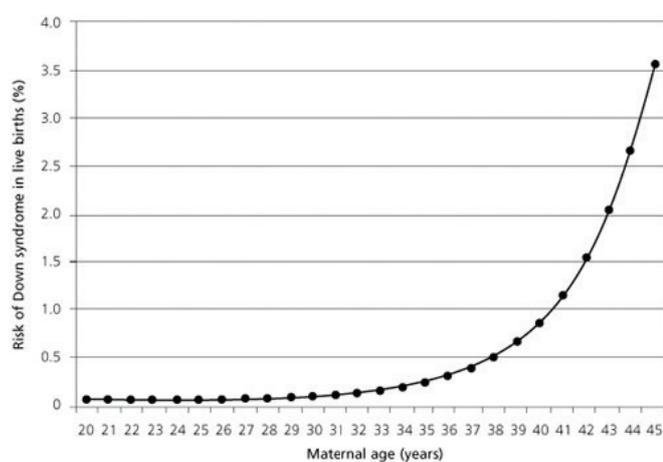


Figure 2 - a graph illustrating the effect of maternal age on risk of conceiving a child with Down's Syndrome

DS entails a set of very similar physical and mental characteristics for those who have it, albeit with some variation. Few people exhibit all the features, and some only exhibit a few. Some physical characteristics include shortness, a small head and ears, short neck, flat facial features, bulging tongue, upward slanting eyes, atypically shaped ears and low muscle tone. They tend to have more flexible joints, drier skin and sparser hair. The most consistent features are the facial appearance, skeletal structure leading to shorter stature and developmental anomalies of the heart. Those with DS are also more likely to develop visual and aural impairments and are at an increased risk of leukaemia and Alzheimer's disease. [NIA, 2017]. People with DS have an increased risk of cardiac disorders, most of which are congenital i.e. present from birth. Congenital cardiac disorders are present in around 40-60 percent of babies born with DS [PASCALL, 2015]. These are mainly septal defects, where part of the heart has not developed properly resulting in a hole being present. The most common congenital cardiac disorder in people with DS is an atrioventricular septal defect (AVSD). It occurs when the septum (partition) between the two ventricles of the heart and between the two atria of the heart does not develop properly and a hole is present. This means blood can mix from the left side to the right side of the heart. As a result, deoxygenated and oxygenated blood mix so the blood circulating the body has a lower level of oxygen, causing further health problems including Eisenmenger syndrome. Many of these heart defects require surgery very early on in the child's life, and

until recently this was not known, hence why much fewer infants with DS survived beyond a few years of age. Because of their prevalence, screening for these issues must happen at a very young age. These problems, whether immediately life threatening or not, must be medically reviewed consistently.

Individuals with DS notably have behavioural and mental features as a result of their genes. These learning disabilities mean that it takes longer for them to develop certain skills, however level of ability certainly varies from person to person. Some typical behavioural attributes to DS can include a short attention span, poor judgment, and impulsive behaviour. Notable mental characteristics are delayed speech and language development, together with slow learning. What makes learning slower is a combination of factors including difficulties with receptive language and short-term memory, together with expressive delays. This means that academic, social and personal skills take longer for people with DS to develop, and most will never entirely reach that of someone without DS. These learning difficulties can be explained by the effect the extra chromosome has on the development of the brain. At a macroscopic level, variations can be seen in certain brain pathways. An example of this is the anterior commissure, a band of nerve cells connecting the two temporal lobes of the cerebral hemispheres across the midline of the brain, which are important for processing visual information and memory (see Figure 3). These appear smaller in those with DS, due to underdevelopment. In addition, the brain is made up of millions of nerve cells (neurons), which communicate with their neighbours through small outgrowths known as dendrites. The number and quality of these dendrites is what determines the level of processing and learning ability of the brain. In a person with DS, abnormal dendritic processes can be seen at a microscopic level. [NEWTON, 2004]. Despite the differences of the brains of those with DS, in the past the impairment of learning ability has been overemphasised, and full potentials have only been realised in recent years due to an access to adequate education, and widespread societal acceptance. It is certainly true that people with DS tend to have specific strengths regarding learning. It is said they have a distinct preference for visual learning, tending to be quite sharp with visual processing. They also tend to have high capacity for empathy and social understanding. They offer more comfort and support in times of distress in others. [KASARI, 2003]

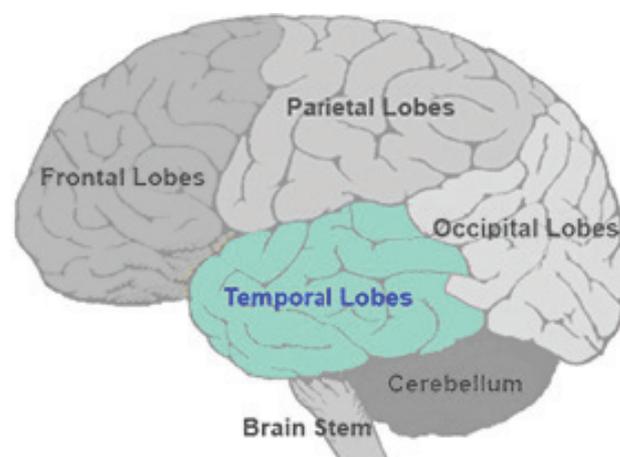


Figure 3 - diagram highlighting the temporal lobes of the brain

The genes of those with DS are the same as everyone else's, just with an extra 1%. This is a very small amount in comparison to the whole human genome, meaning that all the rest of the genetic information is the same

as it would be if the person did not have DS. [KESLING, SAWTELL, 2002]. This extra information gives the potential rise to characteristics of DS, hence why features of those with DS are similar. However, as genes are inherited from parents, people with the condition look more like their family than others with DS.

Given the correct support and education, as it has been shown in recent years, it is certainly possible for people with DS to achieve personal goals and develop sufficient academic and communication skills to live semi-independent lives as they grow up, with full time jobs.

LIFE WITH DOWN'S SYNDROME

Before I address life with DS, I would like to reference a short essay called "Welcome to Holland", written in 1987 by American author and social activist Emily Kingsley about having a child with a disability. It can be found in my references. [KINGSLEY, 1987]. This essay does not encapsulate all that it means to be a parent to a child with a disability, it merely provides a personal and more positive outlook. It shows that it certainly changes one's life, but that does not necessarily mean it changes it for the worse. Kingsley was mother to son Jason, born in 1974 with DS. She and her husband made a real effort to bring up their son in the best way possible, working hard on developing his skills. Jason became the first ever person with DS to appear on television, when he began to feature as a regular guest on *Sesame Street*. This was a big step as it normalised tolerance for a new generation, when he played with other children in a way that acknowledged but did not stigmatise his condition.

People with DS are known for being particularly affectionate and happy, with an excellent outlook on life. In a study approved by the Institutional Review Board of Boston University Medical Centre, 284 people with DS on the mailing lists of six non-profit Down's syndrome organisations around the United States were given a questionnaire on the subject of their lives and wellbeing. Those being surveyed were 12 and older. Among those surveyed, almost 99% of people with DS indicated that they were happy with their lives; 97% liked who they are; and 96% liked how they look. Nearly 99% people with DS expressed love for their families, and 97% liked their siblings. These are some quite heart-warming statistics, and really demonstrate the mindset of those with DS, contented and compassionate and able to really develop loving and special relationships with those around them. As mentioned earlier, those with DS have their own relative strengths. Over time, most teens and adults are competent with self-help and daily living skills which often allows them to lead semi-independent lives, sometimes living by themselves or with roommates. With correct support and ambition, those with DS can strive for personal achievements such as being able to ride a bike, cooking their own meals, going to college, getting a driver's licence, getting married and having a full-time job. Things for people with DS are often done at a slower pace, with more time needed and potentially with a slightly different approach, but this does not make it all impossible. Relating back to the achievements I mentioned at the start, it just shows what is possible.

With regards to the preparation for life – I have mentioned that things are often done slightly differently for people with DS, more support is needed, and they perhaps have different goals to others. While this is true, it is still very important for theirs and others sense of inclusion and acceptance that they are treated like anyone else,

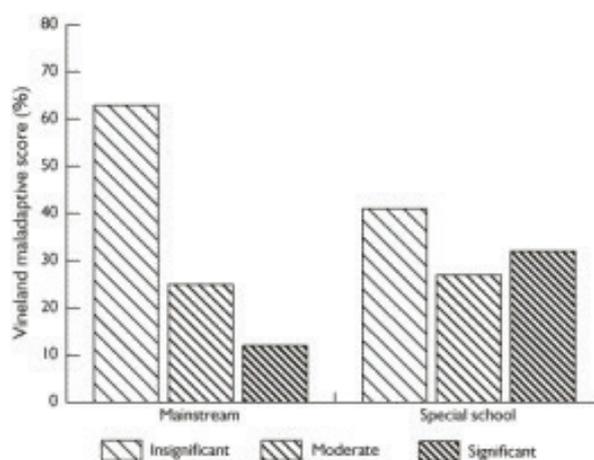


Figure 4 - The significance of reported behaviour difficulties (percentage of teenagers in each category) [BUCKLEY, BIRD 99]

with the same opportunity and freedom. A largescale example of this is with schooling, although all students with DS considerably benefit from having personal learning assistant or a one-to-one. A survey was completed in 1999 which concluded that teenagers with DS educated in mainstream schools are gaining considerable benefits in academic skills, communication skills and social independence [BUCKLEY, BIRD 99]. It was a survey of the progress of 46 teenagers with DS in Hampshire, of whom 18 are in mainstream secondary education and 28 are in special schools. Information was collected on a wide range of issues including, health, behaviour, sexuality and social lives in addition to personal and social independence, communication skills and academic progress. The general trend showed that on average those with DS from a mainstream school were more competent with these tasks than those from the special schools. The surveys were carried out using questionnaires for the parents – the Sacks & Buckley Questionnaire (SBQ) and the Vineland Adaptive Behaviour Scale (VABS). With regards to communication, it was shown that the expressive language of those from the mainstream schools was 2 years and 6 months ahead of the special school group. Some 78% of the mainstream teenagers are rated as being intelligible to strangers compared with 56% in special schools in 1999. This demonstrates that the atmosphere and nurture of mainstream schools provides those students with DS appropriate and more developed communicative skills. They are very inclusive places, those with DS mix with those without and it creates a more equal, rather than separated school community. The other classmates also learn a great amount too, and it provides a valuable and eye-opening experience for everyone else within that school. In addition, the significance of reported instances of difficult behaviour of the children was lower for those from the mainstream schools than the special schools (see Figure 4). It can be seen that difficult behaviour affects the learning and social opportunities of a teenager with DS and can create stress for teachers and families. Contrarily, teenagers who can behave in a socially acceptable and competent manner will be more likely to have friends, have active social lives and to be successful in work as adults.

Some comments on the positive aspects of the teenagers personalities were made from parents involved in the study: "He is popular, friendly and non-judgemental... he has added another dimension to our lives." "Our daughter brings more love, fun and laughter to family life and though she will never be 'academic' there are other qualities she has which cannot be measured." These comments show first-hand the impact



these children have on the people around them.

As shown here with these quotes, there is no doubt that there is a truly special benefit these people with DS give to life for those around them. In a large-scale, population-based study, significantly lower divorce rates were found among families of children with Down syndrome (7.6%) compared with those of children with no identified disability (11.2%). The study involved the families of 647 children with Down syndrome and 361,154 families of comparison children who did not have any record of congenital birth defects (the comparison group). [URBANO, HODAPP 07] This is a remarkable statistic as it shows that something like a disability does not break families apart, but instead seems to bring them closer together. It links quite nicely with the study mentioned before about wellbeing, regarding the statistics about liking family and siblings. It encapsulates the connection within the family and shows that all the things the child brings to the family are valued and cherished.

I was able to contact some parents of children with DS who are part of a local charity my family are involved in via email, in order to gauge more about their view on how having a child with DS has impacted their life. I questioned them on the most valuable thing they had learned from having their child. "Priorities", "Appreciation" and "Love" was what trustee Tatty Bowman told me were the three most important things she has been lucky enough to consider and develop after having and bringing up her son George. She has "no doubt he has made [her] a better person". "It brings a blessed view of life" told Emma Eichhorn, mother to Henry, on the perspective it has given her. Ellie Martin mentioned that the biggest thing she and her family have learned is the "power of acceptance", and the value of embracing what life gives them. (for full responses see Appendix). These truly honest and powerful words I was met with really expresses the eye-opening viewpoint of experiencing first-hand something that is completely different to what people are used to, or what they expected. From this I can learn that despite the challenges raising a child with DS may pose, the initial dread is soon met and replaced by such wonderful qualities, which ultimately lead to a better view on life.

CONCLUSION

When I was 5 years old, my younger sister, Lia, was born and diagnosed with Down's syndrome. Naïve and confused, I did not really know what to make of it, and the idea that my sister was not going to be normal was a complex thought. Until this point, whilst I was aware of disability in the world, I was seemingly ignorant. I was still like this for years to come but as I grew, I learned to understand it all more since I now had the experience in my own household. Life was different at times, yes, and I had many things to learn. Life is spontaneous and changes in an instant but being able to work with what life gives you, figure out new paths and plans is a truly enriching and rewarding experience. It has allowed me to put everything into perspective, appreciate the small things in life and really learn to accept, support and enjoy. While Lia (now 11) is a little different to others her age in some ways, most ways she is just like any other child. She is funny, ambitious, curious and just as annoying as my older sister. I have shared some of my best quality moments with her as we share the same sense of humour and watching her take pride in her own achievements and activities is incredibly special.

I have been curious and fascinated my whole life about this condition, and this project has been an opportunity to really develop my understanding, and research further into the various different aspects of DS. I watched a TED talk performed by Heather Lanier, mother to daughter Fiona who has Wolf-Hirschhorn syndrome; a genetic condition that results in developmental delays. "Good" and "bad" are incomplete stories we tell ourselves' was the title. She talks about what she has learned from having her daughter. She says Fiona has "rare blueprints" and is not designed to be like other people. Life is not factory perfect and genetic flaws are inevitable, and most importantly very much part of our world. She was able to drop her misconceptions on what was "good" or "bad", challenging us to stop fixating on solutions for whatever we deem not normal, and instead to take life as it comes. It can be applied for all people with a disability. They are different, yes, but does that mean bad?

I have learned that there are undoubtedly limitations for those with DS and they will almost certainly not have the level of academic or social skills as their peers, and they may find it harder to develop these skills, but that does not mean that it is not worth the effort. In addition, I have learned about the complexities of the extra chromosome, and what effect it has physically and mentally. It is all accounted for by an extra 1% of genetic information, and the rest is all passed on by the parents just like any other child. This has shown me that indeed there are different characteristics and physical and mental difficulties associated with DS, but that does not make people who have DS any less human, and indeed with their own strengths and support from others, they can lead their own semi-independent lives. Countless successful people with DS can be found all over the internet and there is much evidence for society's changing views. Their condition does not prevent them from getting the most out of life, inspiring others and being a positive and beneficial part of society – and they seem to have a remarkable ability to make people smile. In fact, the world learns a lot from these individuals, which is often overlooked. The same could apply to all people with disabilities, mental and physical. When we learn to accept and understand difference, we learn to value it, rather than judge or criticise. I have learned that everything people with DS bring to this world; all the lessons, love, enjoyment, determination and attitude, makes their life every bit as worth living as mine or yours.



Figure 5 - Sienna (left), Lia (centre), Theo (right) at Bodiam Castle



A theoretical conversion of a Boeing 737800 Jet to Battery Power with respect to Power Requirements and Aerofoil Design

Chris Ratcliffe

OVERVIEW

In this project I calculated the minimum power and energy requirements for flight of a Boeing 737800 airplane with the aim to investigate if an electric conversion is possible and what changes to the wing design would be necessary. This involved:

- Two methods of calculation
- Review of limitations
- Research into power supply
- Redesign of aerofoil

Firstly, by calculation, I found flight velocity for minimum power usage which resulted in a power requirement for level flight at cruising altitude to be 7.91 MW and required power for the climb phase to be 14.7 MW. Therefore, for a flight from Cork Ireland to London Stanstead with a 15 minute climb and 15 minute cruise, the jet would need batteries with energy density 270 Wh/kg. However, after research of current battery technology this energy density is not yet achievable. Although, these calculations had many assumptions including 100% efficiency, standard atmosphere conditions, constant mass and most importantly a hugely approximated climb phase.

For greater accuracy, I used a numerical method to calculate power requirements for the climb phase of a flight, which resulted in an overall reduction in energy requirement over the flight from Cork to London Stanstead. With this improved calculation method, I found a battery energy density of 221 Wh/kg was necessary which is well within current Lithium Ion battery capability.

Finally, with a reduction in cruise velocity required to minimise power usage a new wing had to be designed with a greater lift coefficient to produce more lift with a lower velocity. I modelled this on a software called Xfoil and designed a wing with lift coefficient greater than 1.02 which was required by the lower velocity.

Within my assumptions I can conclude that the conversion of the Boeing 737800 to battery power is theoretically possible for short flights with current battery technology.

However, practically I believe battery technology is still far off the requirements that a real-world situation would demand.

INTRODUCTION

Around the world the aviation industry produces around 2% of all man-made carbon dioxide emissions. A round trip from New York to London produces the same emissions as powering a residential home for a year per passenger. Air Transport Action Group, ATAG, a nonprofit organisation with members including Airbus, Boeing, Rolls Royce and CFM have the goal to cut net aviation carbon emissions by 50% by 2050. In order to meet this target all major players in the aviation industry will have to make significant developments into renewable flight. [1]

I will be investigating the possibilities and limitations of converting a Boeing 737-800 jet (B7378) into a battery powered plane to be used for the flight from Cork Ireland to London Stanstead. The 737 is the bestselling commercial aircraft in the history of aviation. At the start of this year Boeing had over 7000 orders for the 737NG's and the 800 model made up 70% of those orders [2]. With all major airports in the world equipped to hold the 737's it seemed logical to investigate a widely used aircraft. I chose the flight from Cork to London Stanstead because it is one of the only current regular flights of the Boeing 737800 to the UK due to the Corona virus outbreak. Furthermore, it is a relatively short flight at only 59 minutes [3]. Being a shorter flight, it gives the battery powered concept the best chance of success as the technology is still primitive compared to what would be required for flights halfway around the globe.

POWER REQUIREMENTS

{See App.A for larger graphs and data}

T	– Thrust
D	– Drag
V	– Velocity
P	– Power
ρ	– Air Density
S	– Wing plan Area
C_{D_0}	– Drag Coefficient
C_L	– Lift Coefficient
e	– Oswald Efficiency number
AR	– Aspect Ratio
W	– Weight
E	– Energy
GPE	– Gravitational potential energy

In order to calculate the energy requirements and specifications of the necessary batteries capable of powering a B7378 I first calculated the power needed for each part of the flight [4].

For level flight at a constant velocity;

$$\begin{aligned} T &= D \\ P &= T \times V \\ P &= D \times V \end{aligned}$$

The drag component can be split into two: parasitic drag and induced drag. Parasitic drag is drag due to friction between the air and surface of the plane and is defined as;

$$D_{para} = \frac{1}{2} \rho V^2 S C_{D_0}$$

Induced drag is the drag due to lift on the wings and is defined as;

$$D_{ind} = C_L^2 \left(\frac{1}{\pi e A R} \right)$$

In level flight;

$$C_L = \frac{W}{\frac{1}{2} \rho V^2 S}$$

Therefore, induced Drag in level flight;

$$D_{ind} = \frac{W^2}{\frac{1}{2} \rho V^2 S} \left(\frac{1}{\pi e A R} \right)$$

And so, to calculate total drag;

$$D_{Tot} = \frac{1}{2} \rho V^2 S C_{D_0} + \frac{W^2}{\frac{1}{2} \rho V^2 S} \left(\frac{1}{\pi e A R} \right)$$

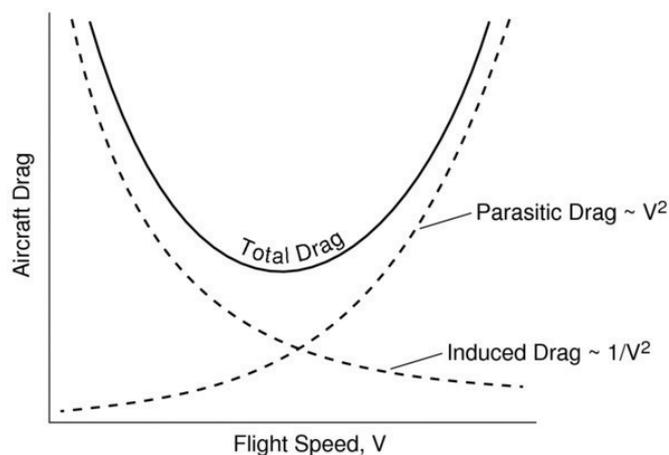


Figure 1, Graph showing Drag against Aircraft speed [4]

Figure 1 shows how total drag and its two component factors vary with flight speed and how there is an optimum speed of V for minimal drag.

Since;

$$P = D \times V$$

The Total power required for level flight is defined as;

$$P_{Tot} = \frac{1}{2} \rho V^3 S C_{D_0} + \frac{W^2}{\frac{1}{2} \rho V S} \left(\frac{1}{\pi e A R} \right)$$

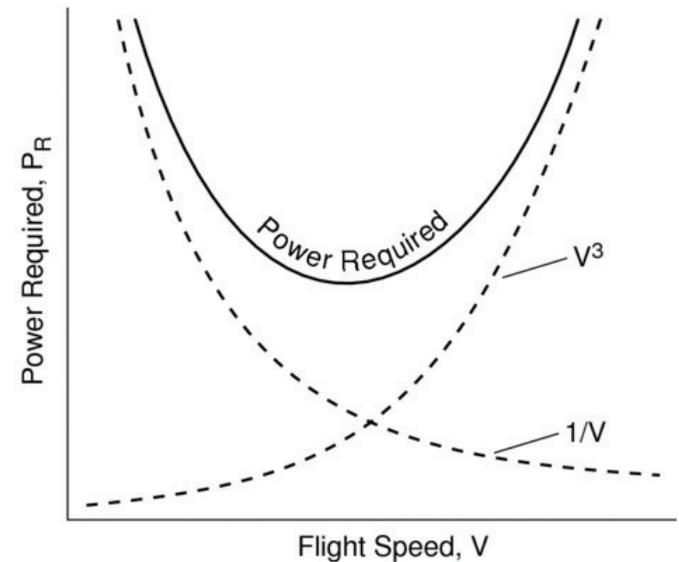


Figure 2, Graph showing Power required against Aircraft speed [4]

Figure 2 shows us how the power required for level flight varies with flight speed. The minimum stationary point is therefore the minimum velocity required for level flight and can be found by the following calculation;

$$\frac{\Delta P_{Tot}}{\Delta V} = \frac{3}{2} \rho V^2 S C_{D_0} - 2 \frac{W^2}{\rho V^2 S} \left(\frac{1}{\pi e A R} \right)$$

Let;

$$\frac{\Delta P_{Tot}}{\Delta V} = 0$$

$$0 = \frac{3}{2} \rho V^2 S C_{D_0} - 2 \frac{W^2}{\rho V^2 S} \left(\frac{1}{\pi e A R} \right)$$

$$V_{MinPower} = \left[\frac{4}{3} \frac{W^2}{S^2} \frac{1}{\rho^2} \frac{1}{C_{D_0}} \left(\frac{1}{\pi e A R} \right) \right]^{\frac{1}{4}}$$

APPLICATION

I split my calculation into two sections, the cruise phase and climb phase. I am assuming an idle descent where no engine power is required in order to minimize the required energy storage to optimise the possibility of battery use. Furthermore, I am assuming no wind, constant mass, i.e. no fuel consumption, and 100% engine efficiency.

I used the following data [2][3][6][7][8], which are published specifications for the B7378.

Mass aircraft (Max T/O weight)	70535 kg
g	9.81 N kg ⁻¹
W	691948 N
Wing plan area, S	124.58 m ²
Air density at sea level	1.225 kg m ⁻³
Relative density at 12km	0.2546
ρ	0.312 kg m ⁻³
Oswald Efficiency, e	0.755
Aspect Ratio, AR	9.54
Drag Coefficient, CD ₀	0.016
Cruise Altitude	12000 m

Table 1, Base data for power calculations

Using data in table 1, I calculated the velocity for minimum power needed for the cruise phase, level flight at 12000m, as;

$$V_{MinPower} = 185 \text{ ms}^{-1} \text{ (3sf)}$$

Hence;

$$P_{Req} = 7.91 \text{ MW}$$

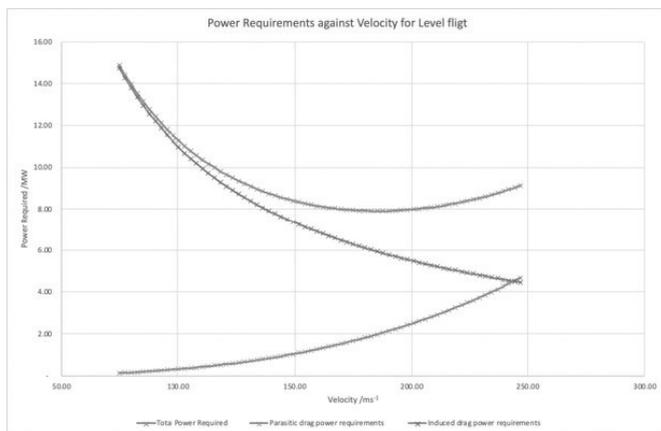


Figure 3, Graph showing calculated power required against aircraft speed

Figure 3 matches closely the predicted curve for the power equation validating the data I have used for my calculations.

For the climb phase I approximated the power requirements as power required to lift the mass of the plane to 12000m in 15 minutes using;

$$GPE = mg\Delta h$$

$$P = \frac{E}{t}$$

$$P = 9.23 \text{ MW}$$

And power required for level flight at average altitude:

Average altitude – 6000m

Relative density at 6000m – 0.5389

Air density at 6000m, ρ – 0.660 kg m⁻³

$$V_{MinPower} = 127 \text{ ms}^{-1}$$

$$P_{Req} = 5.44 \text{ MW}$$

$$P_{ClimbTot} = 14.7 \text{ MW}$$

Using the required power for climb and cruise I can calculated energy needed for a flight with cruise time 1 hour and climb 15 minutes

$$E = P_{Req} t$$

$$E_{Climb} = 13200 \text{ MJ}$$

$$E_{Cruise} = 28500 \text{ MJ}$$

$$E_{Tot} = 41700 \text{ MJ} = 11600 \text{ kWh}$$

THE POWER SUPPLY

Currently all commercial passenger planes around the world are powered by combustion engines, predominantly fuelled by jet fuel, which is a kerosene grade of fuel suited for flight due to its low freezing point of -47° C. Hydrocarbon fuel is so widely used due to its incredibly high energy density; jet fuel has an energy density of 42.8 MJ/kg [9]. Therefore, despite the inefficiency of the combustion engine huge amounts of power can be generated from the fuel.

The B7378 carries 26000L of fuel at max take-off weight [2] which at a density of 0.804 kg/l means the mass of fuel is 21000kg. Therefore, in my theoretical conversion of the B7378 to electric power the total mass of batteries must be less than 21000kg.

With these parameters the greatest limitation on the feasibility of this conversion will be the energy density of the batteries used.

Battery	Energy Density Wh/kg
Lead Acid	40
Nickel Cadmium	65
Lithium Ion	114-247

Table 2 [10][11]

From table 2, it is clear the lithium ion battery configuration has the highest energy density of all current practical battery technology. There are many different forms, however, the most common are LiCoO₂ or the NMC lithium ion battery (LiNi_xCo_yMn_zO₂, where x, y and z vary dependant on the total sum of the others). The Tesla model 3 2170 cell is the current best rated lithium ion cell with an energy density of 247 Wh/kg.

When looking at my desired example flight from Cork to London Stanstead, I calculated for a climb and short cruise time of 15 minutes each [3];

$$E = P_{Req} t$$

$$E_{Climb} = 13200 \text{ MJ}$$

$$E_{Cruise} = 7100 \text{ MJ}$$

$$E_{Tot} = 20300 \text{ MJ} = 5650 \text{ kWh}$$

This equates to a required energy density of 270 Wh/kg.



From calculations above I plotted cruise time against required energy density of battery, assuming:

- 15-minute climb
- Cruise altitude 12000m
- Idle decent

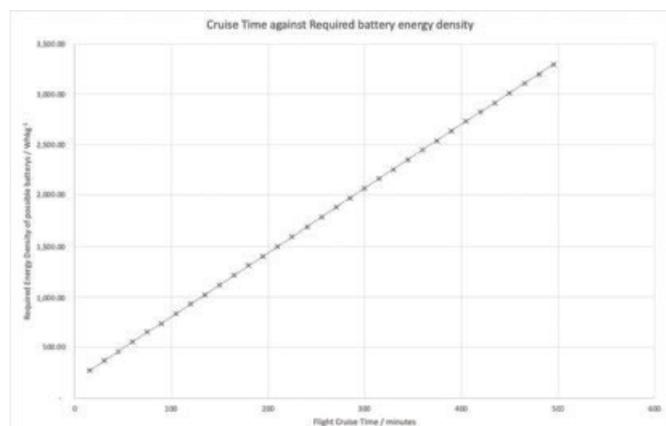


Figure 4, Graph showing required battery energy density against cruise time

From figure 4 it is clear that current battery technology limits significantly the range of an electric B7378. A flight of 4 times the cruise time (60 minutes) of the flight from Cork to Stanstead requires a battery of energy density of 550 Wh/kg which is over double that for the 15- minute cruise.

Even taking into account 100% engine efficiency, no further drag or extra safety requirements for a fly around, an approximated climb phase and idle descent, from my calculation current battery technology would not be capable of powering a B7378 for even a short flight from Cork to London Stanstead.

There is increasing battery research into future battery technology as fossil fuels and the combustion engine become less acceptable.

The amount of research into solid state and lithium sulfur has increased rapidly. As shown in figure 5 they are the second and third most researched battery technologies behind only Li ion, which is reaching its theoretical limit.

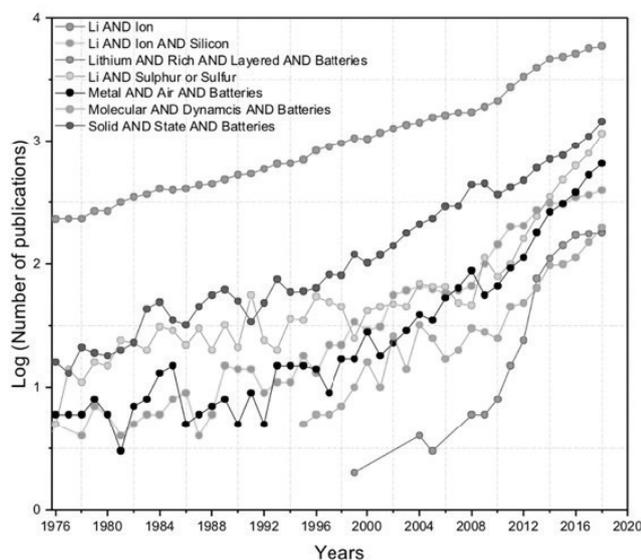


Figure 5, Number of publications with keywords in title of abstracts against year from 1976-2018 [10]

With future batteries there should be a significant improvement to performance and in particular to energy density.

Future Battery	Predicted/Theoretical Energy Density Wh/kg
Solid State Lithium Metal	>300
Lithium Sulfur	2500
Metal Air	11000

Table 3 [10][12]

Using the data in table 3, I could calculate the possible cruise time each type of battery technology could provide by calculating the total energy stored in 21000kg of the battery. Using previous calculations for power requirements;

$$E_{Tot} = E_{Density} \times 21000kg$$

$$E_{Cruise} = E_{Tot} - E_{Climb}$$

$$t_{Cruise} = \frac{E_{Cruise}}{P_{ReqCruise}}$$

Solid state Li Metal - >19.98 min

Lithium Sulfur – 6.17 hours

Metal Air – 28.73 hours

My calculations have shown that with predicted future battery technologies, a plane of size similar to the Boeing 737800 could theoretically be powered by batteries, potentially creating clean commercial flight all the way around the globe.

LIMITATIONS

To simplify the calculations I have done there are many approximations that I will address now as follows:

100% ENGINE EFFICIENCY

I have assumed that all the energy supplied by the batteries will be directly transferred into thrust. While electric motors are much more efficient than combustion engines, they are not quite 100%. There is still energy loss through friction between parts, sound and thermal energy produced by the batteries themselves.

PERFECT FLYING CONDITIONS

I have assumed that no head wind or tail wind is affecting my plane, of course a tailwind would help the batteries increase the range of the aircraft, however, a headwind would be detrimental to the performance of the batteries as drag forces increase. However, a headwind could increase lift as the airspeed over the aerofoil is faster possibly reducing the power requirement for lift.

ENGINE DESIGN

I have assumed that the engine when powered by batteries will still produce the same amount of thrust as when powered by a combustion engine. However, a jet engine relies on the compression of about 20%



of the airflow by the combustion components, which would not be possible without the combustion of jet fuel. In reality an electric plane would most likely have numerous propellers producing thrust to reduce drag and unnecessary weight. But I have not taken this into account.

WAVE DRAG

Wave drag occurs when airflow over the wing is supersonic (faster than speed of sound) which creates sonic shocks breaking the airflow boundary layer on the camber of the wing, however this will not occur under the critical Mach number, M_c , for the plane. Even then the wave drag remains relatively small until Dragdivergence Mach number, M_{DD} , is reached when it rapidly increases the drag coefficient. [5]

NB. Mach number is a ratio between true airspeed and speed of sound at that altitude.

M_c is the lowest Mach number at which airflow over the plane reaches the speed of sound but not exceeding it.

M_{DD} is the Mach number at which wave drag rapidly increases from this point on.

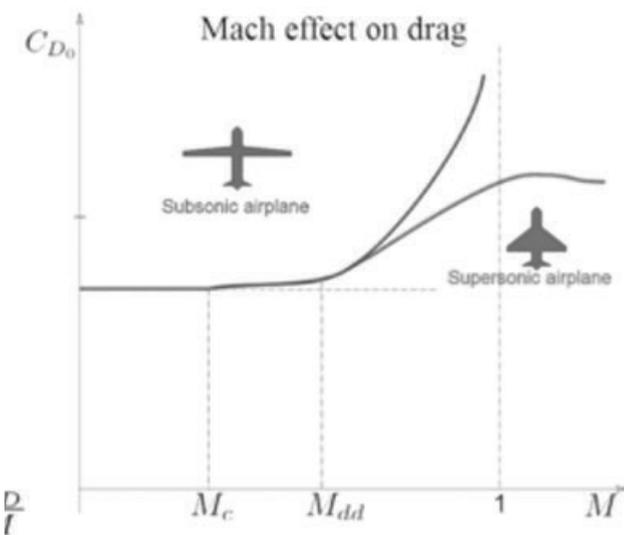


Figure 6, Graph showing effect of Mach number on wave drag [5]

Figure 6 shows how below the critical Mach number M_c for a subsonic plane like the B7378 wave drag remains negligible until M_{DD} . For the B737800 [13];

$$M_c = 0.6$$

$$M_{DD} = 0.8$$

From my previous calculations the optimum cruise velocity for B7378 is 185 ms^{-1} .

Speed of sound at 12000m, a is 295 ms^{-1} [6]

$$M = \frac{V}{a}$$

Mach number at cruise;

$$M_{Cruise} = 0.627$$

As

$$M_{Cruise} < M_c < M_{DD}$$

Wave drag can be ignored as negligible.

CLIMB PHASE

My calculations for the climb phase of the flight rely heavily on major approximations of the power requirements. It also ignores the acceleration on the runway completely, which will be one of the most power intensive phases, as the plane must accelerate the quickest and is in the densest air at sea level so parasitic drag is at its highest.

NUMERICAL MODEL

{See App.B for larger graphs and data}

To better approximate power required for the whole flight I split my climb phase into 4 further parts: runway, initial climb, secondary climb, tertiary climb. [3][14]

This will improve my model as the conditions of the flight change constantly throughout the climb, so the more parts it is split into the better.

I will calculate the power required at each phase of the flight to know the max power required by combining the power to accelerate the plane and power to climb in each phase. I can then use this to sum the energy required in each phase of the flight and hence find required energy density of a possible battery to be used over the whole flight.

For the 4 climb phases I will use a numerical method to find the power. For the cruise in level flight I can use my previous calculation;

$$P_{Cruise} = \frac{1}{2} \rho V^3 S C_{D_0} + \frac{W^2}{\frac{1}{2} \rho V S} \left(\frac{1}{\pi e A R} \right)$$

PHASES OF CLIMB

Runway

- Altitude 0 m
- Rate of climb 0 ms^{-1}
- Velocity 0 – 80 ms^{-1}
- Time 0.5 minutes
- Acceleration 2.67 ms^{-2}
- CL 1.09

Initial Climb

- Altitude 0 - 305m
- Rate of climb 1.69 ms^{-1}
- Velocity 80 - 85 ms^{-1}
- Time 3 minutes
- Acceleration 0.03 ms^{-2}
- CL 1.09

Secondary Climb

- Altitude 305 – 4600 m
- Rate of climb 14.32 ms^{-1}
- Velocity 85-150 ms^{-1}
- Time 5 minutes
- Acceleration 0.217 ms^{-2}
- CL 0.40



Tertiary Climb

- Altitude 4600 – 12000 m
- Rate of climb 18.97 ms⁻¹
- Velocity 150 – 180 ms⁻¹
- Time 6.5 minutes
- Acceleration 0.09 ms⁻²
- CL 0.4

In addition, my equation for power had to be modified as previously I had assumed no acceleration and the only force opposing the thrust as drag, in level flight. However, now as shown in figure 7, I must consider the component of weight in the direction of flight and the power required to accelerate the plane.

- α – Angle of attack
- γ – Angle of climb
- V – Velocity direction vector
- F – Force direction Vector
- Mg – Weight of aircraft
- D – Drag force vector

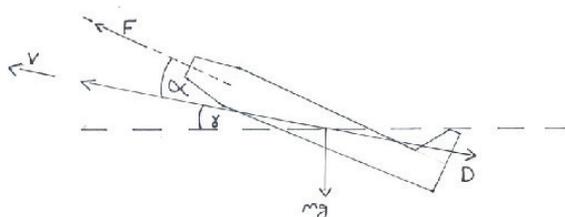


Figure 7, Diagram showing component forces acting on climbing aircraft [5]

$$\sum F = ma = F\cos(\alpha) - D - mg\sin(\gamma)$$

However, α is often less than 10° [5] so;

$$\cos(\alpha) \approx 1$$

And;

$$F = D + mg\sin(\gamma) + ma$$

$$D = D_{Ind} + D_{Para}$$

To find the power required I plotted a graph of drag against velocity and GPE against time and found the area under and gradient of the line respectively. Using a numerical method with values as shown under the phase headings and constants used previously, I calculated force required at various time intervals using;

$$F = \frac{1}{2} \rho V^2 S C_{D_0} + C_L^2 \left(\frac{1}{\pi e A R} \right) + m(g\sin(\gamma) + a)$$

Where ρ was found by interpolation along a graph of relative air density against altitude.[6]

GPE was calculated using;

$$GPE = mgh$$

ANALYSIS

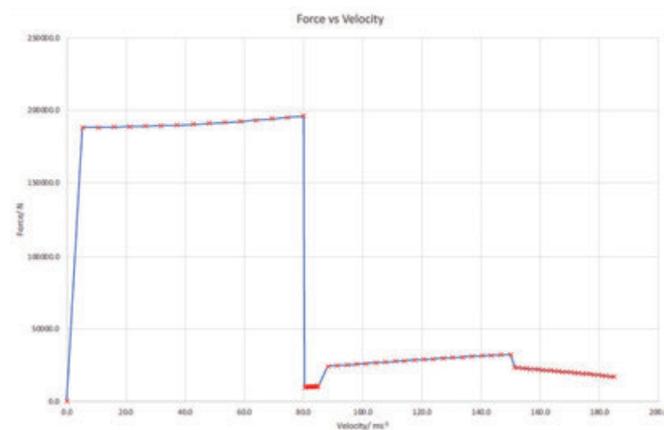


Figure 8, Graph showing Force against velocity

To calculate the area under figure 8, I used the trapezium rule by interpolating force values using a velocity interval of 1 ms⁻¹. Results of this are in table 4.

The graph is separated due to the force required to accelerate the plane (ma term in the equation), as I assumed different constant accelerations for each phase.

	Power to accelerate	
Runway	14.58	MW
Initial	0.14	MW
Secondary	1.82	MW
Tertiary	0.72	MW
Cruise	7.91	MW

Table 4, Power to accelerate the plane

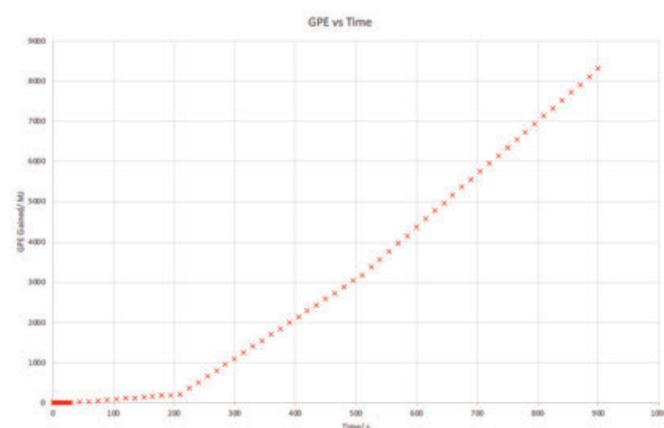


Figure 9, Graph showing change in GPE vs Time

I calculated the gradient of each phase of climb from figure 9 to find the power required to lift the plane to 12000m. Results for this is shown in table 5.



	Power to climb	
Runway	0.00	MW
Initial	1.17	MW
Secondary	9.91	MW
Tertiary	13.13	MW
Cruise	0.00	MW

Therefore, the total power required for flight;

	Total power	
Runway	14.58	MW
Initial	1.32	MW
Secondary	11.73	MW
Tertiary	13.85	MW
Cruise	7.91	MW

Table 6, Total power of whole flight

From table 6, the max power output of a battery used would have to be 14.58 MW as the power to accelerate the plane on the runway is the most power intense phase of the flight.

For the flight from Cork to London Stanstead, of climb 15 minutes and cruise 15 minutes the total energy requirements are;

	Energy for Cork to Stanstead	
Runway	437	MJ
Initial	237	MJ
Secondary	3519	MJ
Tertiary	5402	MJ
Cruise	7120	MJ
Total	16716	MJ

Table 7, Energy requirements for exemplar flight

From table 7, converting from MJ to kWh, the total energy for the flight from Cork to Stanstead is 4643 kWh, which with 21000kg of batteries would need a battery of energy density 221 Wh/kg. This is within current battery technology limits. My numerical model has produced a smaller value for the power required in the climb phase of the flight than my previous calculation which I believe to be more accurate within my parameters.

Therefore, within my assumptions I can conclude that the conversion of the Boeing 737800 to battery power is possible for short flights alike Cork to London Stanstead with current battery technology. However, practically I believe battery technology is still far off the requirements that a real-world situation would demand.

AEROFOIL DESIGN

{See App.C for graphs and data}

The B7378 is designed to cruise at about 230 m/s however to reduce power consumption based on figure 3, I determined that the electric converted plane would cruise at 185 m/s for most efficient power use.

The required lift coefficient of the wing at $\alpha = 0^\circ$ (level flight) can be calculated using;

$$C_{LReq} = \frac{W \cos \gamma}{\frac{1}{2} \rho V^2 S}$$

Using data from table 1;

$$C_{LReq} = 1.02$$

However, I must ensure the drag coefficient of the wing remains at 0.016 or less to ensure no more power is required to overcome drag.

To design this wing, I used a software called Xfoil [15]. This allowed me to create an aerofoil and produce pressure polars to give the lift, drag and moment coefficients of the wing and the terminal point.

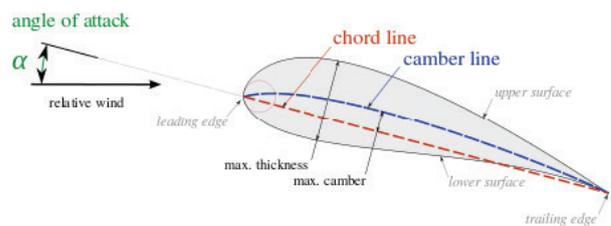


Figure 10, Aerofoil diagram

I started with the NACA wings [16] developed by NASA in the 1920's and changed, max camber, max thickness and position along the aerofoil of max camber and thickness.

For example, the NACA 2210 wing, has max camber 0.02 at $x = 0.20$ and max thickness 0.10 at $x=0.30$, I adjusted these variables to understand their effect on lift drag ratio.

From this I found moving the max camber towards the trailing edge will increase the lift drag ratio. Moving the max thickness towards the trailing edge can reduce the drag however has little effect on the lift drag ratio.

Increasing camber will increase the lift drag ratio and changing thickness has little noticeable effect. Although I did find that a thinner leading edge allows for a better lift drag ratio.

Xfoil can calculate for viscous liquids so I calculated the Reynolds number and mach number for the plane at cruising altitude [17].

$$\text{Reynolds} = 1.19 \times 10^6$$

$$\text{Mach} = 0.44$$

I used the NACA 5330 wing as a base for my final design. (See appendix C for earlier iterations)

Final Design	Base wing NACA 5330		
Max Camber	0.01	at x =	0.32
Max Thickness	0.15	at x =	0.29

Table 8, Final Wing geometrics designed on Xfoil

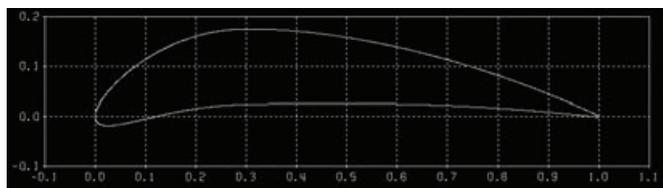


Figure 11, Designed aerofoil

Calculated polar for: e-B7378

1 1 Reynolds number fixed		Mach number fixed					
xtrf =	1.000 (top)	1.000 (bottom)					
Mach =	0.440	Re =	1.190 e 6	Ncrit =	9.000		
alpha	CL	CD	CDp	CM	Top_Xtr	Bot_Xtr	
0.000	1.0268	0.01576	0.00904	-0.1923	0.3470	0.0345	

Table 9, Output of Xfoil calculations

This shape aerofoil, in figure 11, provides a C_L greater than required at 1.027 and has the drag coefficient, C_D , of 0.0157. Which is equal to the value of C_D for the original wing 0.016.

The top and bottom xtr values in table 9 indicate where boundary layer separation occurs along the aerofoil, this is called the terminal point. Boundary layer separation is the separation of laminar airflow from the surface of the aerofoil into turbulent flow. The closer to the trailing edge this occurs the less drag experienced by the wing. [5]

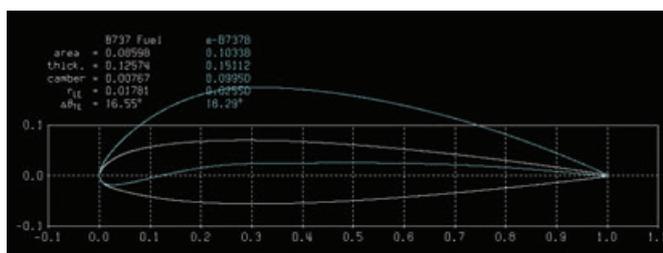


Figure 12, Overlay of real and my design of aerofoil {18}

Figure 12, Overlay of real and my design of aerofoil {18} Figure 12 shows my designed aerofoil in blue and the actual B7378 aerofoil in white. It has a much higher camber than the original B7378 wing. This allows for higher lift as a higher air pressure can build on the bottom edge as shown by the pressure polar, figure 13. This polar is reversed to have the pressure of the upper side at the top. However, the upper side has lower negative pressure. The greater the difference between the upper and lower curves the more lift is created.

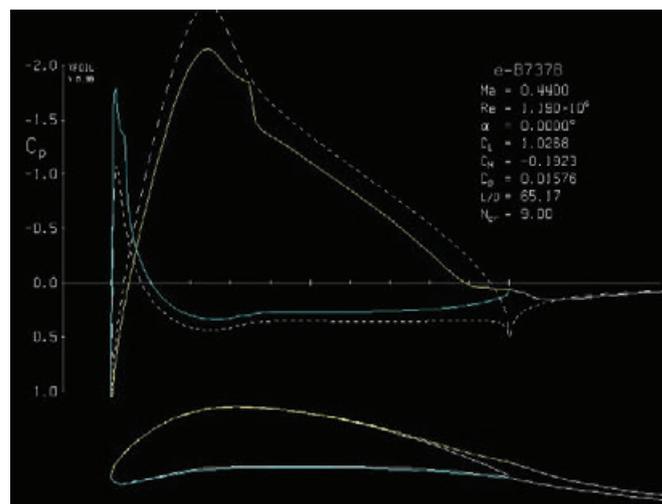


Figure 13, Pressure polar for alpha = 0

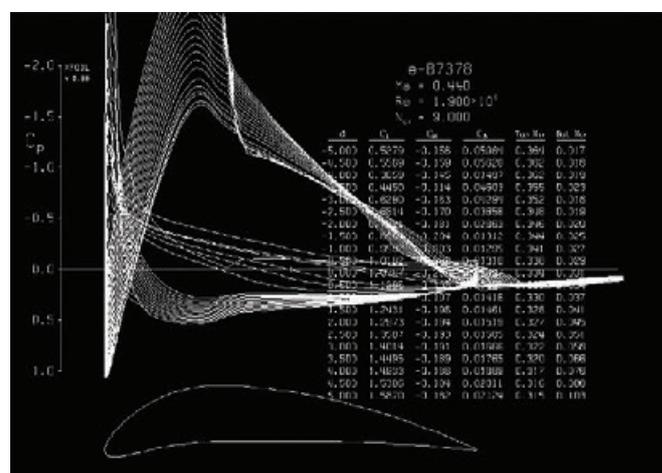


Figure 14, Pressure polar for alpha = -5 to 5 in 0.5 degree steps

When comparing the lift and drag coefficients at varying angles of attack, as shown in figure 14, the highest lift drag ratio of 70.4 is achieved at $\alpha = 1.5^\circ$. Showing that my aerofoil is most efficient at $\alpha = 1.5^\circ$, however will still function at a required standard when in level flight. By plotting a C_L against α graph I can find the angle of attack for max lift and at what angle stall occurs. Stall is a loss of control caused by flow separation from the boundary layer on the upper surface of the aerofoil. As angle of attack increases the air pressure on upper surface decreases until separation occurs. [5]

From figure 15, $C_{Lmax} = 2.016$ at $\alpha = 14^\circ$, beyond this point C_L decreases, this is where stall occurs. As most commonly $\alpha < 10^\circ$ stall should typically not be a problem for my wing.

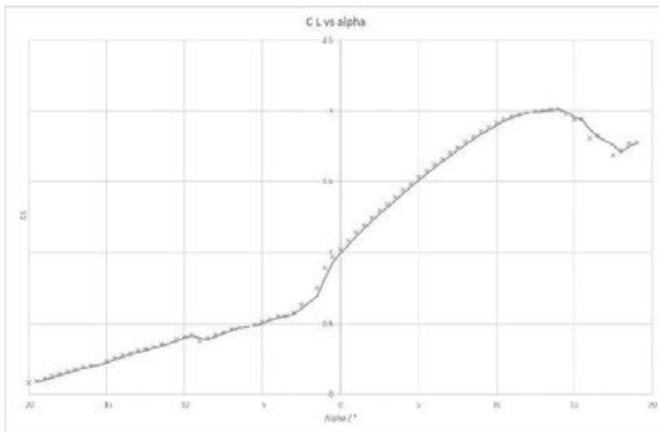


Figure 15, Graph showing C_L against α

My aerofoil design is for the midspan of the wing only and so root and tip aerofoil modelling would also be required along with redesign of all aerodynamic surfaces. This would include the tail and fin but also flaps and ailerons among other moveable aerodynamic parts.



APPENDIX

C: AEROFOIL DESIGN

Iterations:

No.1 – Base shape NACA 2210, adjusted

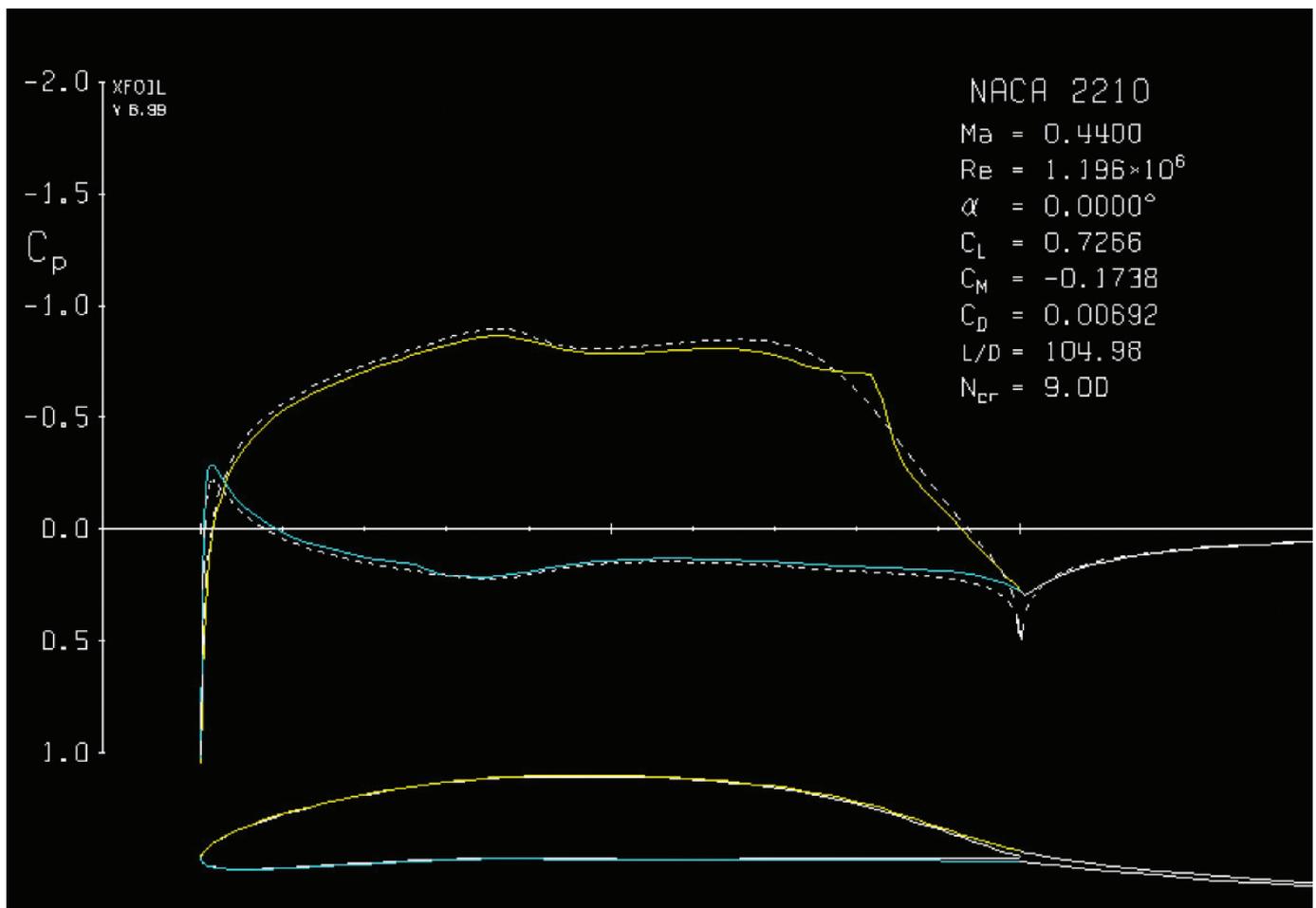
Calculated polar for: NACA 2210

1 1 Reynolds number fixed

Mach number fixed

xtrf = 1.000 (top) 1.000 (bottom)
 Mach = 0.440 Re = 1.196 e 6 Ncrit = 9.000

alpha	CL	CD	CDp	CM	Top_Xtr	Bot_Xtr
0.000	0.7266	0.00692	0.00224	-0.1738	0.8230	0.2595



No.2 - Base shape NACA 7410, adjusted

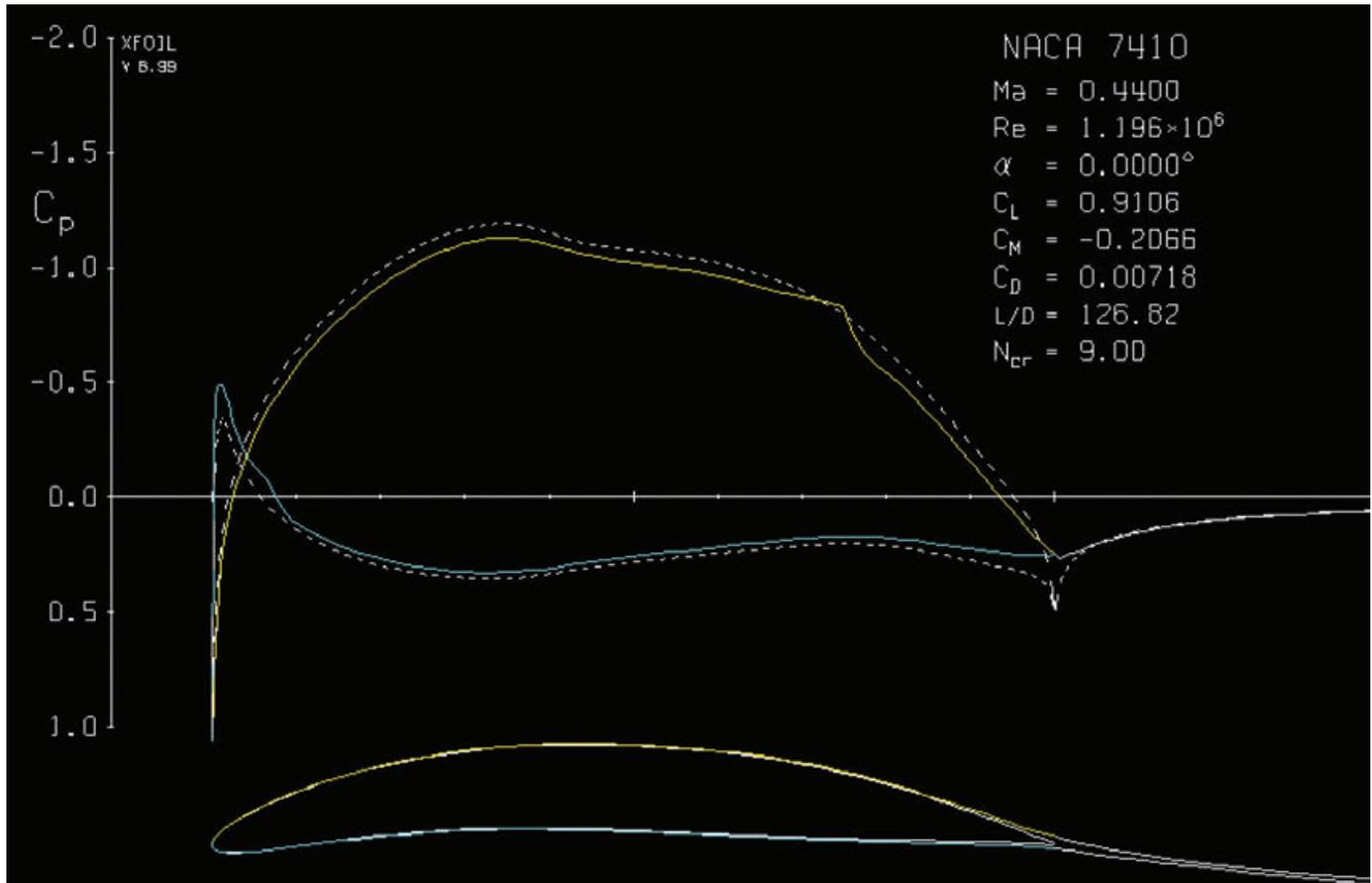
Calculated polar for: NACA 7410

1 1 Reynolds number fixed

Mach number fixed

xtrf = 1.000 (top) 1.000 (bottom)
 Mach = 0.440 Re = 1.196 e 6 Ncrit = 9.000

alpha	CL	CD	CDp	CM	Top_Xtr	Bot_Xtr
0.000	0.9106	0.00718	0.00189	-0.2066	0.7469	0.0717





No.3 - Base shape NACA 5330, adjusted

Calculated polar for: NACA 5330

1 1 Reynolds number fixed

Mach number fixed

xtrf = 1.000 (top)

1.000 (bottom)

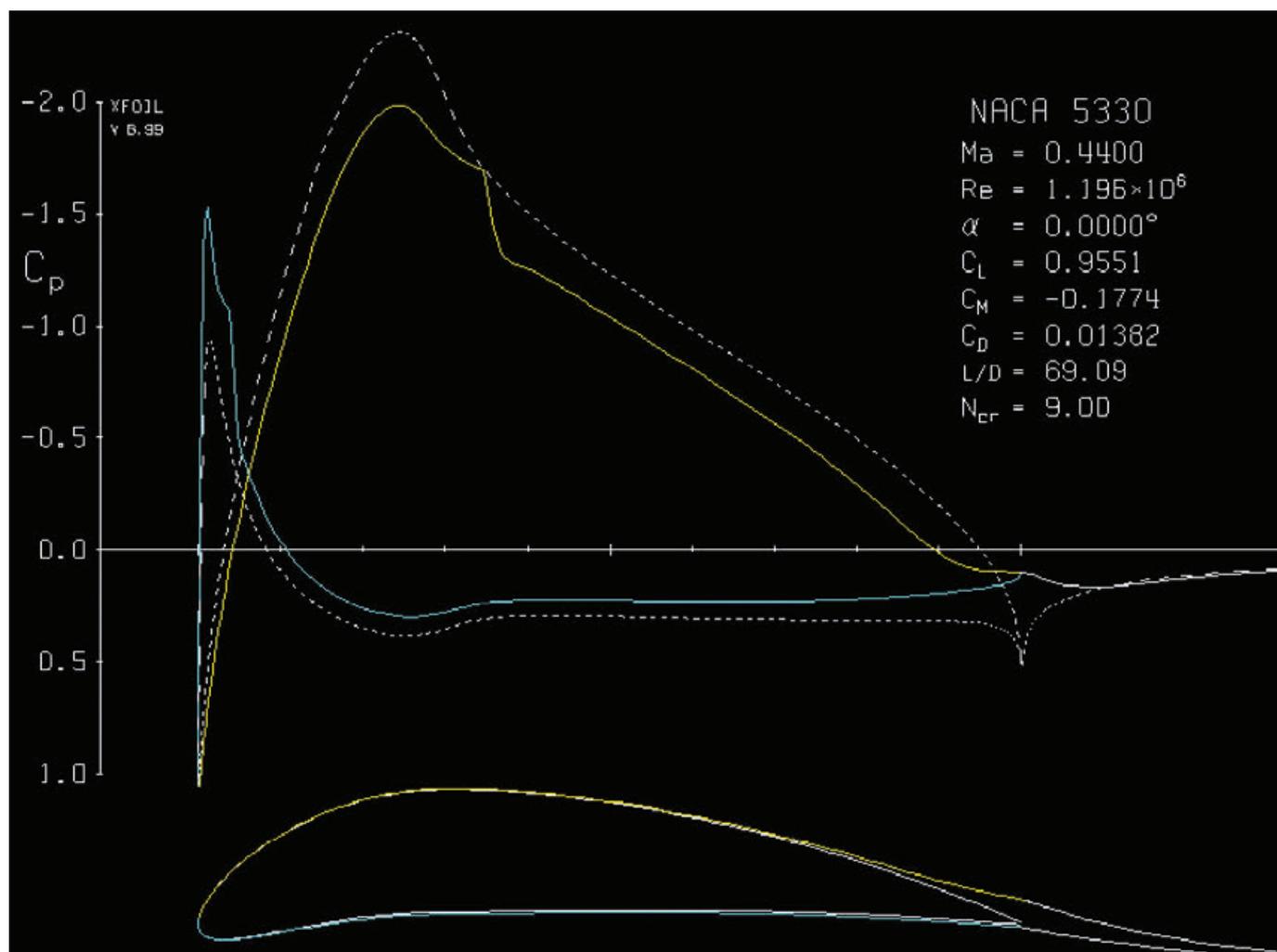
Mach = 0.440

Re =

1.196 e 6

Ncrit = 9.000

alpha	CL	CD	CDp	CM	Top_Xtr	Bot_Xtr
0.000	0.9551	0.01382	0.00686	-0.1774	0.3501	0.0393



Final Design – eB7378, base aerofoil NACA 5330

FIGURE 10

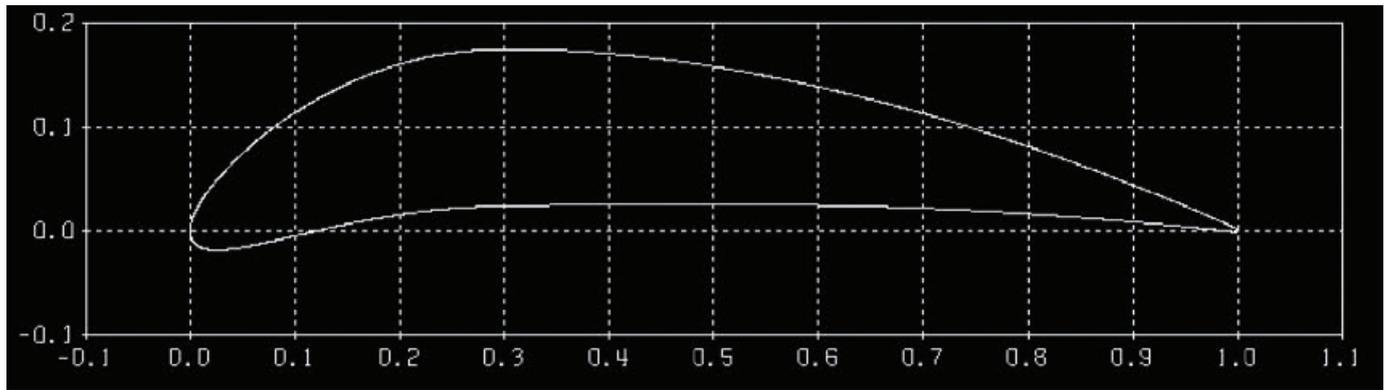


FIGURE 11

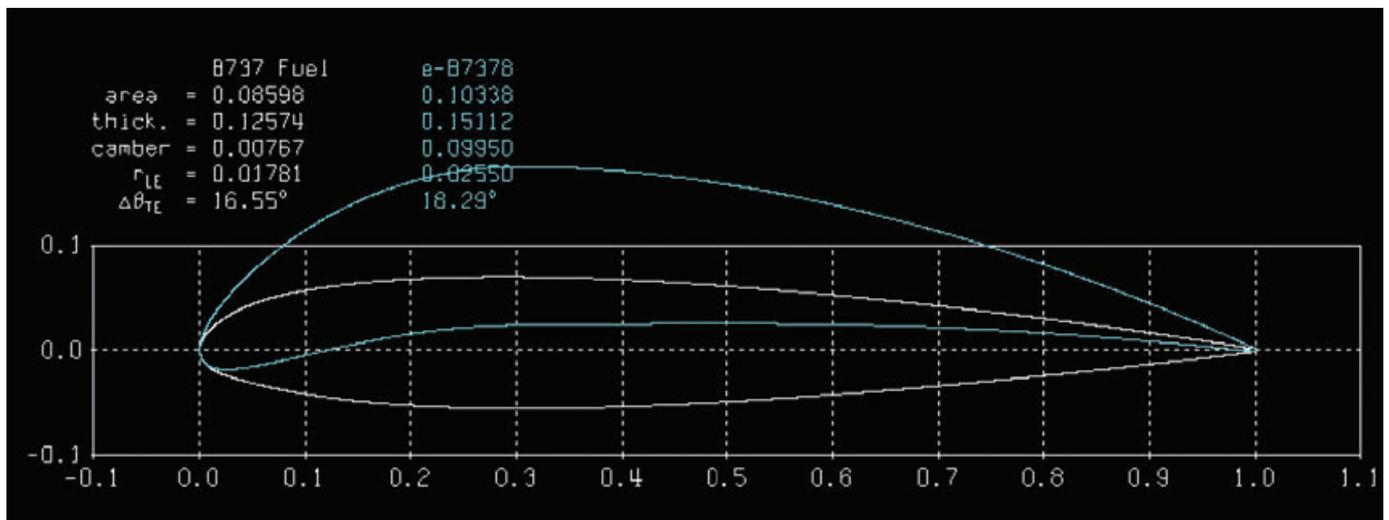
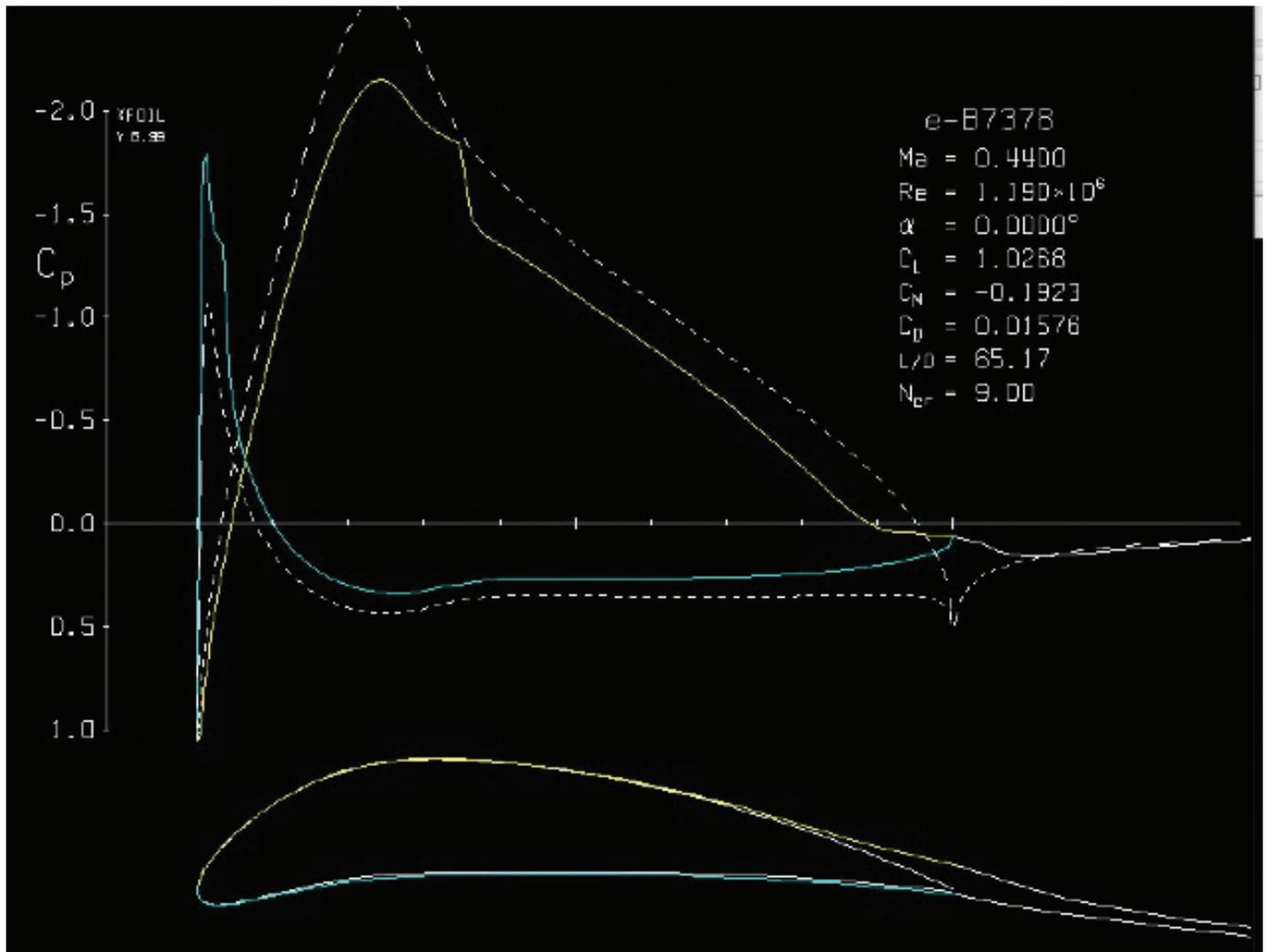




FIGURE 12



Calculated polar for: e-B7378

1 1 Reynolds number fixed

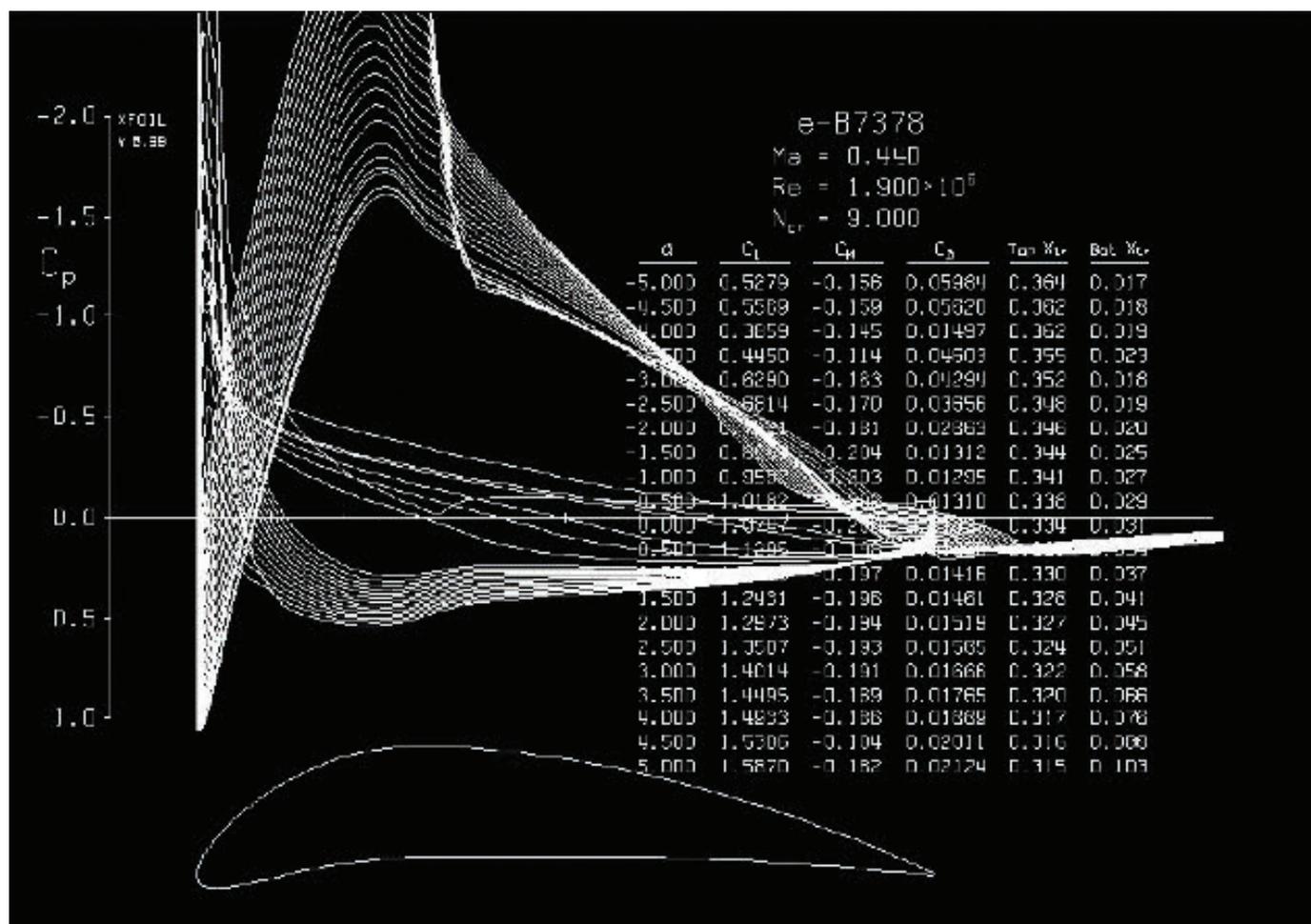
Mach number fixed

xtrf = 1.000 (top) 1.000 (bottom)
 Mach = 0.440 Re = 1.190 e 6 Ncrit = 9.000

alpha	CL	CD	CDp	CM	Top_Xtr	Bot_Xtr
0.000	1.0268	0.01576	0.00904	-0.1923	0.3470	0.0345



FIGURE 13



Calculated polar for: e-B7378

1 1 Reynolds number fixed

Mach number fixed

xtrf = 1.000 (top)

1.000 (bottom)

Mach = 0.440

Re =

1.190 e 6

Ncrit = 9.000

alpha	CL	CD	CDp	CM	Top_Xtr	Bot_Xtr
-5.000	0.5171	0.06238	0.05826	-0.1509	0.3908	0.0211
-4.500	0.5376	0.05708	0.05294	-0.1571	0.3851	0.0223
-4.000	0.5517	0.05330	0.04917	-0.1556	0.3791	0.0225
-3.500	0.5586	0.05068	0.04658	-0.1510	0.3752	0.0229
-3.000	0.5829	0.04760	0.04349	-0.1504	0.3707	0.0239
-2.000	0.6808	0.03815	0.03383	-0.1600	0.3620	0.0265
-1.000	0.9144	0.01563	0.00932	-0.1952	0.3555	0.0300
-0.500	0.9729	0.01555	0.00902	-0.1941	0.3514	0.0321
0.000	1.0268	0.01576	0.00904	-0.1923	0.3470	0.0345
0.500	1.0838	0.01604	0.00926	-0.1910	0.3450	0.0372
1.000	1.1400	0.01641	0.00961	-0.1898	0.3428	0.0403
1.500	1.1945	0.01693	0.01012	-0.1883	0.3404	0.0442
2.000	1.2465	0.01762	0.01080	-0.1866	0.3380	0.0486
2.500	1.2961	0.01850	0.01168	-0.1847	0.3355	0.0537
3.000	1.3425	0.01956	0.01277	-0.1825	0.3325	0.0601
3.500	1.3877	0.02074	0.01399	-0.1802	0.3299	0.0678
4.000	1.4373	0.02176	0.01507	-0.1786	0.3285	0.0777
4.500	1.4852	0.02289	0.01629	-0.1769	0.3268	0.0908
5.000	1.5308	0.02419	0.01768	-0.1749	0.3249	0.1063



ORIGINAL POLARS

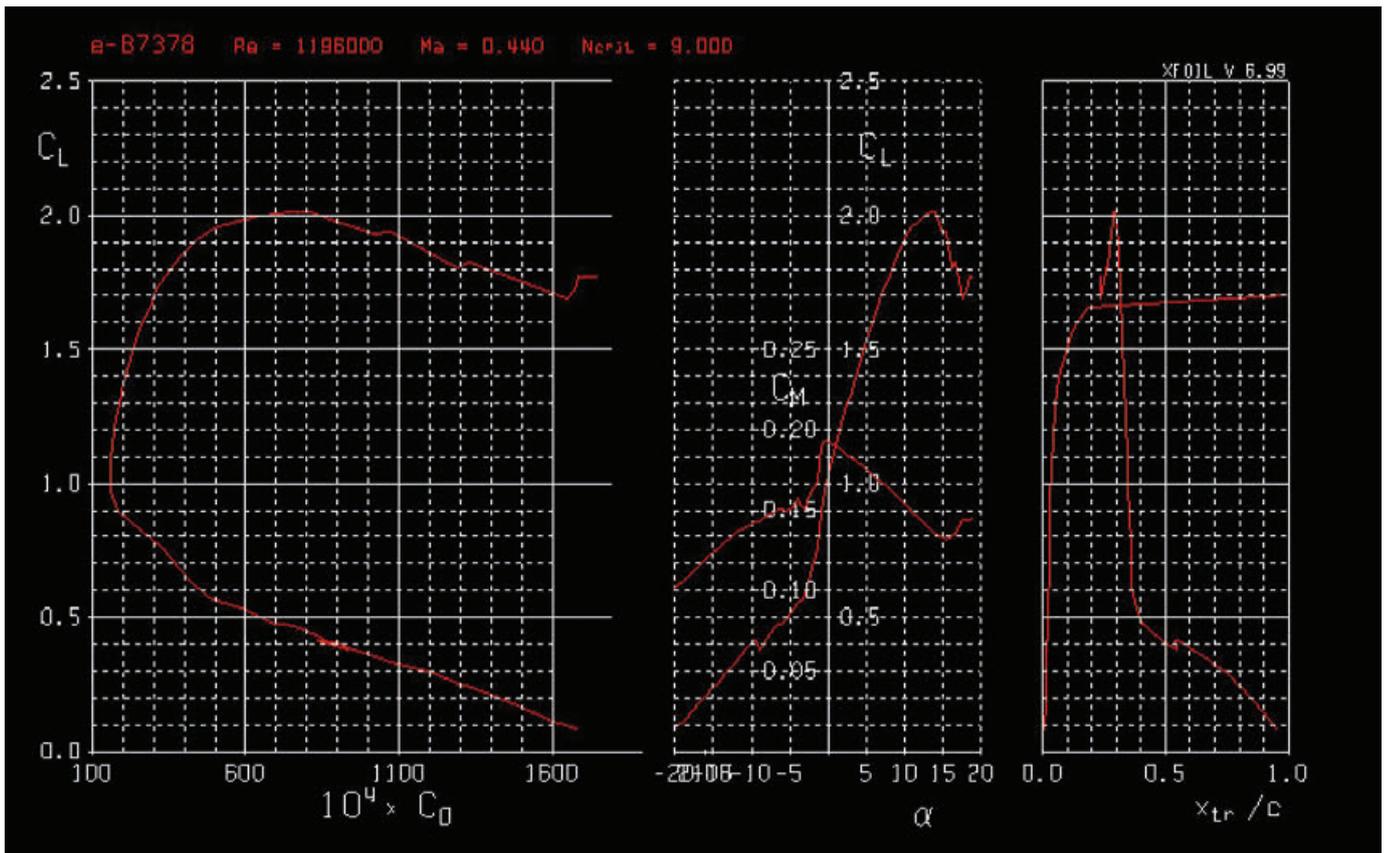
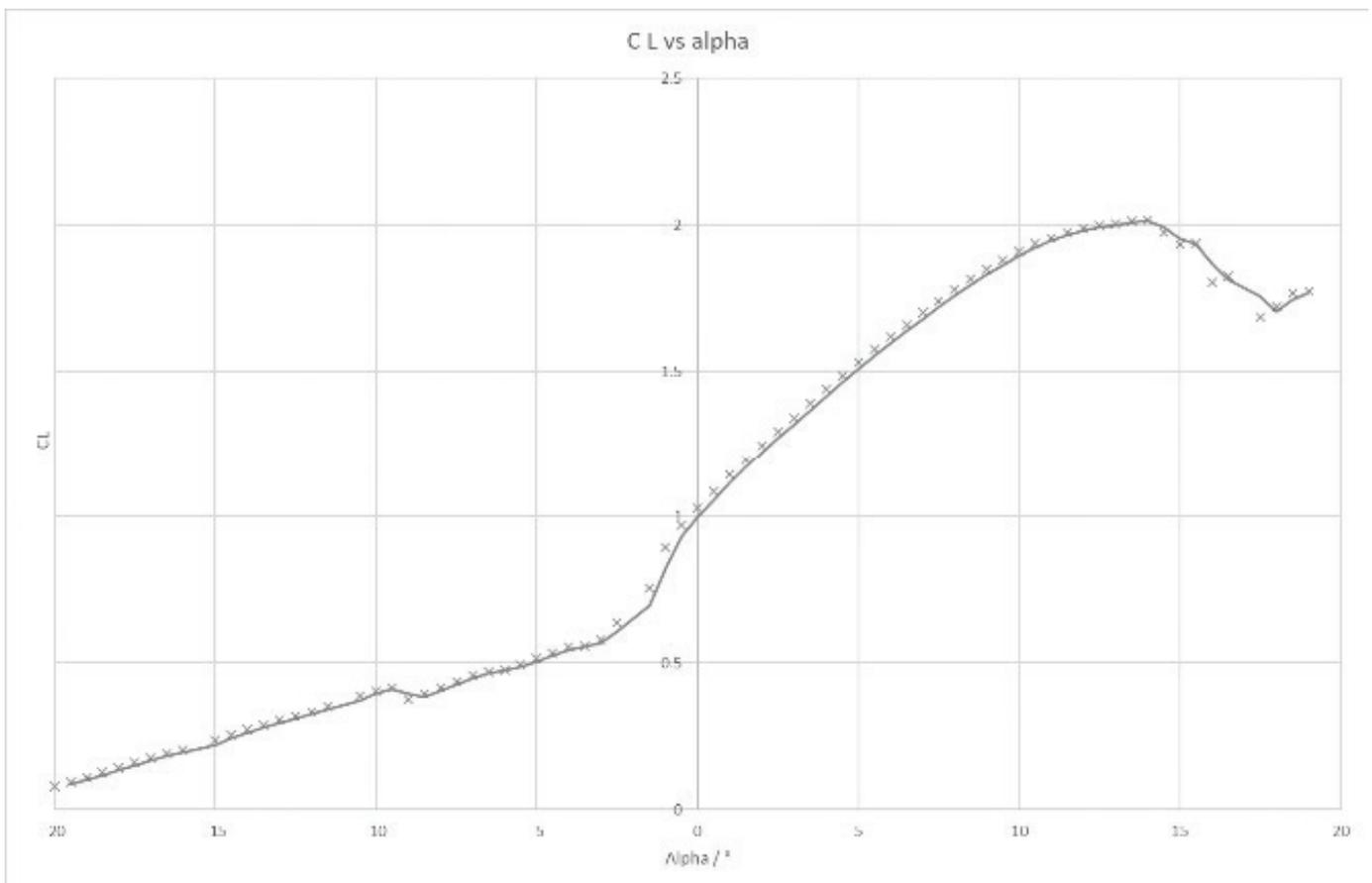


FIGURE 14



Analysing the Gacha Mechanism: The truth behind the rates

Muhammed Hussain

PREFACE

It was nearing the deadline for submitting the title for your IIA and I had still not given the project much thought. Forcing myself to choose a topic on the final day of the extended deadline, I was deliberating going down one of two routes; the easy yet laborious, or the difficult but enjoyable. After taming down my ambitions I went with the former and submitted that in thinking the route would be less bumpy.

Fast forward a couple of days and I am at my desk looking at my blank screen titled, "How Immigration affects the Local Economy." Finally I come to the realization that this is going to be a reading fest, examining 30 odd articles and picking out what is relevant for me, only to come up with a conclusion that mirrors someone else's with data that has been sourced from some one else. What would be my input? Besides, the title itself was bland and monotonous, exactly not what I wanted to my IIA to encompass.

So, I had to start from scratch with Mr Bradford thinking I was some labour economist. This time I decided I would go down the other route titled: "Are in-app purchases a scam?" Being a frequent app gamer and statistics enthusiast, I thought this was the perfect idea until I became aware of its potential downfall: the countless different app genres and in-game purchase functions. For example, in one game "gems" might be spent trying to summon a character from a pool, in another "stones" may merely speed up time. Trying to make comparisons of the value of in-game currency between two distinct games (whose currency served different functions) would be very difficult, let alone quantifying the value of speeding up game time itself.

With the help of Mr Xuan I managed to narrow down my appetite to a more specific genre, gacha: the controversial Japanese lootbox¹ extraordinaire now common in western app stores and perhaps the biggest "socially approved" scam out there. Having played these games before and having previously meddled with statistics in the context of these games, I realized there was a much bigger section of this topic to be explored using more elements of statistics, I at the time did not know of.

I wanted my IIA to be truly independent, in other words, I wanted most of the research to be my own, using my own unique methods and coming up with my own conclusions about these games. That's why choosing such a niche topic that had not been previously explored, bar the odd superficial statistical analysis by players in the games' communities, was perfect for my goal.

However, there were two large problems that I immediately faced as I tried to change subject from in-app purchases as a whole to the specific genre of gacha. Firstly, gacha was too specific and foreign a genre that many people did not understand the complicated terminology associated with it. Being an avid gacha gamer myself did not help either, as it was difficult to gauge what a stranger to the game would

not at first understand. In fact, after submitting my first draft for approval, those who had played such games prior to reading my draft had good things to say about it, as opposed to those who hadn't who struggled to get past the first couple pages. To fix this, I decided to restructure my IIA so it was more easy to follow, add a definitions page for any foreign vocabulary, buff up the introductory explanation of gacha, and finally add footnotes to parts that may not be fully accessible to a lay reader. This came with a downside in that my essays' word count ballooned to make up for the more detailed explanations.

The second problem was perhaps the bigger of the two. Having already written a large amount for my old topic of in-app purchases it was painful to cut out the now irrelevant sections. Changing topics immediately made the vast proportion of my then IIA redundant. My over attachment to what I had previously written made it difficult to cut stuff out on the basis of forcefully made reasons explaining their relevance. This resulted in an IIA which lacked a coherent structure and clearly looked as if someone had changed ideas halfway through writing it. In the end I managed to overcome this issue with the help of Mr Xuan (...again), by planning my new essay and only extracting the relevant parts from my old IIA, editing them slightly before inputting them into my new one.

The end product was an IIA dipped in statistical analysis, coated with behavioral analysis with a sprinkle of scorn on top. I understand some of this analysis does not apply to the whole gacha genre, indeed there are some games which are not so much of a scam but more a delight to play. This essay was mainly aimed at targeting the so-called gacha mechanism in popular gacha games that have, in some cases, been criticized as "scam-like" or close to "gambling" by many game critics.

INTRODUCTION

With "92% of mobile games on Google Play free"² as of December 2016, it is not new news that the free-to-download business model is dominating app stores. Rather ironically, its these "free games" that are commandeering the revenue charts with Minecraft, the top paid app, not making the top 100 in terms of gross revenue³. With high profit margins and no fear of piracy, these games meet market desire to pay in sequential small amounts rather than large lump sums from the start. The barrier to play these games is virtually non-existent, being free to download, and they appeal to the large competitive audience through intense multiplayer elements.

What distinguishes this model of games from the other model, (pay-to-download) is the barrier to entry (in the form of upfront costs). With a \$5 price tag, consumers will be hesitant to try the game at all and be more demanding that the experience matches the price. It's a risk consumers don't wish to take unless knowing for certain, through reviews and gameplays, that the game is "worth it." On the other hand, free games are free, at least from the start anyway. It is unusual



for “free games” to stay “free” as people play more and more. Using the absence of a barrier to amass a large player base, the competitive nature of the game begins pulling in money. Relying on the “freemium strategy,” such games are the perfect encapsulation of tricks and devices to edge unsuspecting players to make their first purchase.

However, one branch of “free-to-download” games takes these tricks to another level, so much so that they have been frequently likened to that of gambling and scams. These “Gacha games,” whose purchase-function (a so called “gacha-mechanism,” similar to that of lootboxes) relies so heavily on chance, are breeding grounds for tricks to not only initiate a gambling-like process but to sustain it as players, particularly competitive ones, spend on a weekly basis to try acquiring a new hero which is always, suspiciously, better than the last.

With the old saying at heart: “nothing is free in this world,” in this essay I will be exploring the gacha mechanism, shining a light on the true purposes hiding behind seemingly unsuspecting benefits, serving to lull you into paying the same, if not more for what had previously put you off from downloading another pay-to-download game.

In fact, the extent of the hidden and unsuspecting nature of these ploys, deliberate or a result of convenience, can be demonstrated by this one overlooked factor that already makes any in-app purchase very dangerous; the method of payment. Such a seamless and intangible transaction process (as exists in both Apple and Google Play stores) numbs the “pain of payment” and leads to unbalanced cost-benefit analyses. This in turn leads to overspending on items that the consumer would otherwise be reluctant to buy given a more upfront, physical and persistent payment system.

In a study by Drazen Prelec and Duncan Simester of MIT (2001)⁴, it was found that shoppers spend up to 100% more when using credit cards instead of cash. Similarly in another study, the authors found that participants were willing to spend \$175 to throw a Thanksgiving party when using a credit card to buy the food, but only \$145 when using cash. Why is this the case, and what are the implications for in-app purchases?

As opposed to payments in cash, when purchasing virtual goods by card there is no physical element of exchange. As a result, the reality of the loss, commonly enforced by the handing over of physical money, is not fully realized, downplaying the cost of the item. On the other hand, such a seamless transaction highlights the benefits of the purchase to the consumer via the immediate transfer of the good. Allowing a consumer to benefit from a good immediately after purchase, whilst dampening the “pain of payment” causes a one-sided cost-benefit analysis to occur. Consequently, this unbalanced analysis leads to a greater willingness to purchase the virtual good or service with card than what would be the case for cash. There are numerous studies to support such a notion. In a paper documented by Priya Raghuram and Joydeep Srivastava in 2008 in the “Journal of Experimental Psychology: Applied”, it was concluded that “the more transparent the payment outflow, the greater the aversion to spending or the higher the pain of paying...leading to less transparent payment modes such as credit cards being more easily spent.” In other words, since counting coins is more painful than a simple tap on a screen the period of doubt and regret about such a purchase is prolonged, thereby leading to more considered decisions.

Furthermore, with virtual purchases edging closer towards one-button

authentication systems as well as the stubborn existence of no-refund policies, the threat of impulse buying is growing. Comparing the purchase of in-app products to that of shopping in a grocer: “When consumers encounter vice products - such as cookies, cakes and pies – the emotive imagery and associated desire trigger impulsive purchase decisions. These visceral factors entice them to include such vice products in their shopping baskets, even though they consider such products to be unhealthy. Pain of payment can curb the impulsive responses, and thus reduce the purchase of such vice products.”⁵ By contextualising the phenomena to app markets, we see that the “vice products” are the virtual goods consumers desire although rationally view to be unnecessary (in the analogy “unhealthy”). The existence of such a prompt payment system, which lowers the “pain of purchase,” can cause action out of the impulsive thoughts and wants leading to purchases the consumer would not rationally adhere to.

Finally, a common phenomenon associated with purchases by card, particularly for virtual goods, is “payment decoupling”. Payment decoupling is the process of separating or decoupling a purchase from the consumption and in doing so reduces the perceived cost of the product. Decoupling is particularly present in purchases through credit cards as by postponing the payment by a few weeks and grouping it up with all the other purchases, the payment is separated from the original purchase. This effect has two main consequences. The first is a loss of track of payments as they are made less salient through decoupling. A study composed by Soman (1997) found that students leaving the campus bookstore were much more accurate in remembering the cost if they paid by cash rather than by card: “payment by credit card thus reduces the salience and vividness of the outflows, making them harder to recall than payments by cash or check which leave a stronger memory trace” (p. 9).⁶ This follows on to the other consequence of decoupling: overspending. With lower perceived costs and unfamiliarity with previous purchases it is not surprising that overconsumption or rather careless consumption is a large problem with seamless payment methods such as these. Putting this into context, the use of credit cards can lead to forgetful and underestimated purchases of virtual products which build up over time, as the consumer is removed from the cost and merely focuses on the utility it brings.

Consequently, the implication this has for our gacha games is rather significant. Being dominated by one-tap card transactions, such a payment medium could not be any simpler. This, therefore, can lead to a lower perception of costs especially when people are nearing the checkout for a purchase they are deliberating on whether or not should be bought. In essence buying in-app products is easy, so much so that it can lead to overconsumption and/or consumption of products that wouldn’t be bought given a “harder” transaction system. It is fascinating how something as simple as the payment method, attributed to the final stage of a purchase, can contribute so much to the purchase itself, and begs the question what other overlooked and now deliberate factors heavily determine the final outcome of a purchase?

BACKGROUND INTO “GACHA”

The term “gacha,” originating in Japan and now commonplace in the West, describes a toy machine into which a customer puts money in exchange for a plastic egg acquired through the twisting of a crank.





Figure 1: A picture of a Japanese gacha vending machine housing many different collectible toys. [asle](https://www.asle.com/)

Inside the egg is usually a collectible (often figurines) which is part of a completable set. Gacha games are apps that virtualize the gacha mechanic, using a virtual currency in place of real money.

"In these phone games, there are usually a variety of cards, characters, units or other items that players can collect (that often have functions in-game) most of which, if not all are only obtainable via the gacha mechanism. Hence players, "pull" or "spin" the gacha (analogous to the capsule-toy vending machine) using a specific amount of in-game currency to receive, from a pool, a randomized unit.⁷

The gacha mechanism itself is essentially the process of obtaining characters from the general pool in accordance with publicized rates and chances.

WHY ANALYSE THIS MECHANISM?

Well, the gacha mechanism is notoriously successful with the gacha industry generating \$55 billion since 2007.⁸

Not only that, but this model has frequently been compared to that of collectible trading card games as well as gambling. In other words, splurging cash on a gacha game (via the mechanism) will not always result in gains, especially since the gacha mechanism operates purely on given rates and chances. Therefore, by taking apart the gacha-mechanism using the help of statistics and behavioral economic principles we will be able to truly see if the genre is, indeed, close to gambling and what lies at the heart of its success.

In order to simplify the situation we will use two in-demand games for reference and example during our analysis.

The first game we will be looking at is called "Naruto Blazing," (by Bandai) themed on the popular anime Naruto. With over 10 million downloads on the Google Play store and even more on the Apple store, it has amassed a large playerbase over its three years in service. The second game called "Grand Cross: 7DS" is a more recent addition to both markets (having been released on 3rd March 2020). It is again very popular with over 7 million downloads across its Global and Japanese releases. In these games the in-game currency is used, primarily, to summon characters from pools which are updated every week with the addition of a new character.

To smoothen descriptions of Gacha games further down the line, I will now define some vocabulary or terminology that will frequently appear in such descriptions.

The first use of such terminology in following sections will be highlighted in bold text.

Summon – A summon is the act of drawing a character from a banner-specific pool. It is this "summoning" of characters that lies at the heart of the gacha mechanism

Pulls/to Pull – refers to the acquiring of an item/character from a summon

Rank – is a class of characters. In the gacha genre there are three main ranks, R, SR and SSR as defined below. The concept of three summonable classes is the same in all gacha games, differing only by class-names.

Free-to-play player (F2P) – is a player who does not buy or buys very little in-game currency and plays the game simply because they enjoy it.

Pay-to-play player (P2P) – is one who pays on a consistent basis, either from a competitive viewpoint (to maintain a competitive advantage) or simply to unlock more features of a game they enjoy.

Rates – The term refers to the percent chance of a character appearing on a given pull (usually a single). Shortened version of "drop rate."

R – refers to "Rare," and is the lowest ranking of character. They are the body that takes up most of the summoning rates for the sole reason of minimizing the chances for players to get anyone valuable (SSRs). Basically a populous of characters whose presence signifies more of an absence, if anything.

SR – refers to "Super Rare" and is the middle ranking. Characters of SR rank are often useful in some games but in the majority of gacha games they are either fodder for SSR heroes or simply units added to largen the pool.



Figure 2: A typical summoning banner. The featured character is advertised at the top, underneath which there are two options to summon.



[Featured Character Drop Rate]		
Rarity	Character	Drop Rate
5 (Featured)	Minato Namikaze Raikosekka	1.00%

[Drop Rate]		
Rarity	Number of Units	Drop Rate
5(Featured)	1 Units	1.00%
5	77 Units	14.00%
4	41 Units	62.00%
3	15 Units	23.00%

Drop Rate differs depending on rarity

Figure 3: The picture to the left, shows the publicised drop rates for a banner in *Naruto Blazing*, including the featured unit: "Minato Namikaze". In the picture, the number "5" refers to the rank SSR, "4" to SR, and "3" to R.

We can see how the featured unit has a drop rate of 1% as opposed to the other SSR units which only have a 0.18% rate each. (Found by dividing 14% by 77).

SSR – refers to "Super Super Rare" (believe me or not). These characters have the smallest rates of appearance. They are most desired because firstly they tend to be the best units and secondly, since the new weekly character is always an SSR, pulling an SSR potentially means that the new character has been acquired.

Shaft – is a summon in which no SSR was obtained.

Unit – a character or item that is summoned via the gacha-mechanism and has in-game functions.

Banner – A banner is what players summon on. It is where players go to summon for characters. Each banner usually comes with its own new character that is included in a pool with other old characters.

Featured unit – a featured unit is the new character in a banner that has a heightened drop rate compared to other units of similar rank.

Diamonds – The name of the in-game currency for *Grand Cross 7DS*. It may also be used in this essay, for simplicity, to refer to in-game currency as a whole

Pearls – The name of the in-game currency for *Naruto Blazing*

Pity bar – The pity bar is part of the pity system in *Grand Cross 7DS*. After each shaft multi (defined later on) =the pity bar fills up. After 5 shafts the pity bar is full and guarantees the player an SSR in his next multi, (hence the name "pity," as the system is "taking pity" on players with bad luck.)

SINGLES AND MULTIS IN THE GACHA MECHANISM

The gacha mechanism as explained previously is the summoning of characters from a general pool that have in-game uses.

When it comes to gacha games, summoning operates through two different options. The first, known as a "single", is where you summon for just one unit. The second, called a "multi", is where you summon for 10 units in one go. A multi costs the same as 10 singles.



Figure 4: The summoning options: "Multi" and "Single" as seen in *Naruto Blazing*

As you see in Figure 4, in *Naruto Blazing*, a "single" costs 5 pearls and a "multi" costs 50.

In most games there is an incentive encouraging players to summon via the multi. This incentive is in the form of a multi-summon promotion that increases the chances of pulling an SSR and, in turn, the featured unit. This means that, with the multi-summon promotion in effect, a multi no longer has the same rates as the equivalently priced 10 singles. For example, in *Naruto Blazing* the multi-summon promotion is "An SR or higher guaranteed." Without this promotion a multi would be simply be an option of completing 10 'singles' in one go. However with this promotion in play, a multi has slightly better rates than the 10 singles for reasons explored later.¹⁰

In this essay we will analyse three aspects (or potential "scams") of this gacha mechanism that, while may look like benefits from the outside, have underlying purposes and costs to the consumer. They are:

- The low rates.
- The existence of "multis"
- A so called "pity-system,"

SCAM 1: THE TRUTH BEHIND THE RATES

The first aspect of the gacha mechanism we will be analyzing is the low **rates** associated with these games. By referring to the rates on respective **banners** we will be able to ascertain how much the gacha-mechanism costs (by calculating the cost of **summons** needed until a particular banner-**featured unit** is pulled). We will then compare it with



the benefits one receives after having acquired that unit and finally examine the implications this has on F2P players.

EVALUATING THE COST OF THE GACHA MECHANISM

In this section, we will be using the help of statistics to attach a true cost to the gacha mechanism¹¹ by using the given rates to predict the expected amount of summons needed to pull a desired banner-featured unit. From then we derive the cost by converting the price of the summons into a pound value.

[Although multis, because of the added promotion, have a better chance at pulling a unit, we will be using ‘singles’ in our analysis as the added promotions for multis tend to vary between games. In some games there is no promotion at all, in others the promotion is minimal (will be explored later) and in a few the promotion is very good. Thus whilst multis often have better drop rates and thus give lower costs for our gacha-mechanism, ‘singles’ will be a better, more general representation of the genre.¹²]

Singles:

In every summoning banner, there is always a new character (the featured character) whose rates are higher than those of characters of the same rank (SSR). Therefore, the majority of people summoning on the banner are doing so with the hopes of “pulling” the new character. This allows us to assume that each summon has the purpose of acquiring the new character. Hence, once the new character has been acquired, the purpose is fulfilled, and no more summons take place. So we will model how many “singles” are needed to be expected to pull our first copy (of the new character).

The probability distribution used to quantify the probability of doing something for the first time on a particular trial is the geometric distribution

To calculate the probabilities described by the distribution we use the general formula:

$$X \sim \text{Geo}(p)$$

$$P(X=x) = (1-p)^{x-1} p$$

Furthermore, applying the characteristics of a geometric progression we see that:

$$P(X \leq 50) = \frac{p(1-(1-p)^{50})}{1-(1-p)} = 1-(1-p)^{50}$$

From this we can derive the equation for cumulative geometric probabilities for first-time successes on trials greater than a certain number x.

Since $P(X=x) + P(X > x) = 1$, you can deduce that $P(X > x) = (1-p)^x$, and from that $P(X \geq x) = (1-p)^{x-1}$.

With the geometric distribution covered to a sufficient degree, we can move onto applying it in an in-game scenario using the rates in **Grand Cross: 7DS** as an example:

From Figure 5, we see that there is a 0.5% chance of pulling the new (featured) character on each single. In our case the new character is “[Harlequin] King the Fairy King.”

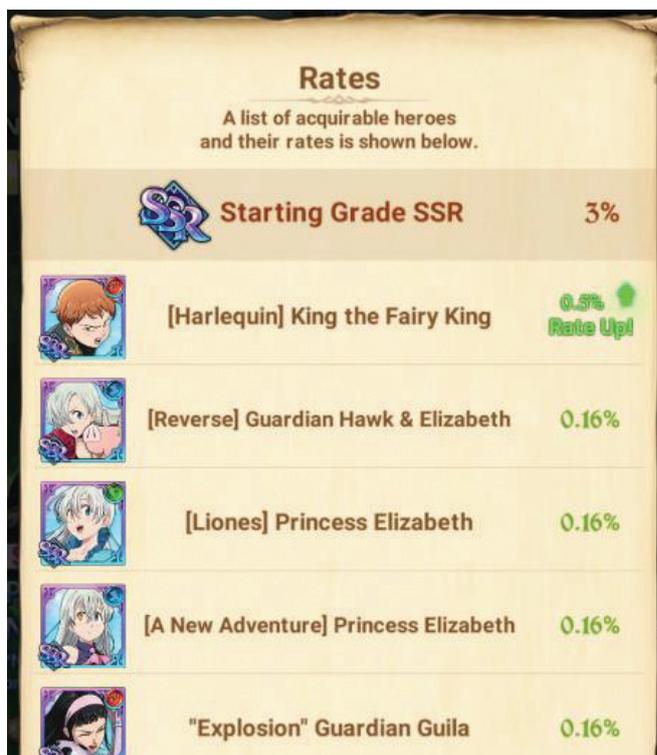


Figure 5: Illustrates the drop rates for a particular banner in **Grand Cross: 7DS**. We see that the featured unit for the banner has a 0.5% drop rate (a rate higher than the other equivalent SSRs in the pool)

Therefore, we can model a geometric distribution of: $X \sim \text{Geo}(0.005)$

This allows us to make the following observations:

There is a 0.005 chance (or 0.5% chance) that a player manages to obtain the character on their first single, costing them merely 3 diamonds.

In the first 10 singles, the chance of a player obtaining his first copy of the new character is:

$$P(X \leq 10) = 1 - (0.995)^{10} = 1 - 0.95111 \dots = 0.0489 \text{ or less than a 5\% chance.}$$

In the first 20, the chance is:

$$P(X \leq 20) = 1 - (0.995)^{20} = 1 - 0.90461 \dots = 0.0954 \text{ or less than a 10\% chance}$$

In the first 50, the chance is:

$$P(X \leq 50) = 1 - (0.995)^{50} = 1 - 0.778313 \dots = 0.222 \text{ or just over a 20\% chance}$$

In fact, we can find the number of trials needed to get a probability above 50%:

$$P(X \leq x) \geq 0.5$$

$$1 - (1-p)^x \geq 0.5$$

$$-(0.995)^x \geq -0.5 \quad (\text{Note that when we divide by } -1 \text{ or any negative number, we flip the inequality sign})$$

$$x \log(0.995) \leq \log 0.5 \quad (\text{Since } \log(1-p) \text{ is a negative number we need to flip the inequality once more})$$

$$x \geq \log_{0.995} 0.5$$

$$x \geq 138.28 \text{ (2.d.p.)}$$



The above working tells us that you need to do 139 singles to at least have a 50% chance of pulling your first copy. In other words, in Grand Cross: 7DS, you are paying 417 diamonds (since each single is 3 diamonds), which costs £308, only to have a 50% chance to pull your desired unit once. Worse still, the mean of the geometric distribution, given by $1/p$, tells us that on average one would expect to pull their first copy of a character after their 200th single (600 diamonds), or after having spent £450.

Therefore, we can say that the gacha-mechanism in Grand Cross 7DS has a cost of £450 as that is the amount players must spend (on average) in order to fulfill the purpose of acquiring the new banner featured character.

EVALUATING THE BENEFITS:

The temporary nature:

Despite such a high price tag, the benefit or utility that comes from spending the £450 is only temporary. In all gacha games, as well as in other loot box games, units always get better as the game matures. Intuitively it makes sense; one needs better characters to have a better chance at completing the harder missions. People would not summon for more units if the units they had were already better. Since summoning lies at the heart of gacha games, such games must stimulate summoning to stimulate revenue, through the constant release of newer and better units, as well as harder missions to accompany them. This in turn results in a sustained deflation of the in-game currency. By realizing that the goods the in-game currency buys are the units themselves and by valuing the units in a certain measure, we see that the value that can be bought with a given amount of currency increases as the game gets older. In essence, the purchasing power of in-game currencies continuously increases as the game releases newer, better characters in banners with the same price and same rates.

To explain our point we will be referring to the character progression in Naruto Blazing over its 3-year lifetime. If we were to look at the first and most recent character side-by-side the obvious difference will

be in their stats (i.e. strength, health, speed, e.t.c). Therefore, if we calculate the average strength of the three newest units and compare it with the average for the three oldest units we should have an estimate for the increase in character quality. However, strength varies between characters and is often traded for damage multipliers. This means a character may have low strength but to compensate for it, a very large damage multiplier. A more realistic comparison should be taken from the damage dealt by each unit in-game, although that too varies between missions and seasonal activities. Thus, a more representative evaluation of the appreciation in character quality can be found simply in the difference in length of the description of their abilities. I call it the Letter Oriented Label Length Operator, or LOLLO for short.

If we take the word-for-word description of the ability of an old character and that of a new, by comparing the number of letters used to make up the respective descriptions, the percentage difference should shed some light on the appreciation of said characters. This use of measure is based on the fact that as the game progresses, character abilities become more complexed and innovative leading to longer descriptions. To remove any bias that will effect our appreciation measure, we have to choose characters of the same rank, in our case SSRs. The word-for-word description of the ability for our oldest unit is: "3.2x attack toward 1 enemy(s) in range." This sentence-long description accounts to 32 letters. On the other hand, the word for word description of the ability of our newest character is: "5x attack toward all enemies in range and knocks them back. 75% chance of speed reduction for 4 second(s), and reduces their Chakra Gauge by 2. Also nullifies damage you receive from Ninjutsu or Secret Techniques for 3 turn(s), and restores own Chakra Gauge by 3." This paragraph-like description numbers to 225 letters, or 7 times as much as the description for our much older character. Using the average letter count for the three oldest characters and the three newest characters, we see that the latter is 5 times longer than the former. This measure helps illustrate, therefore, a fast appreciation of character quality present in these games and thus how much more value the in-game currency can buy as time develops.

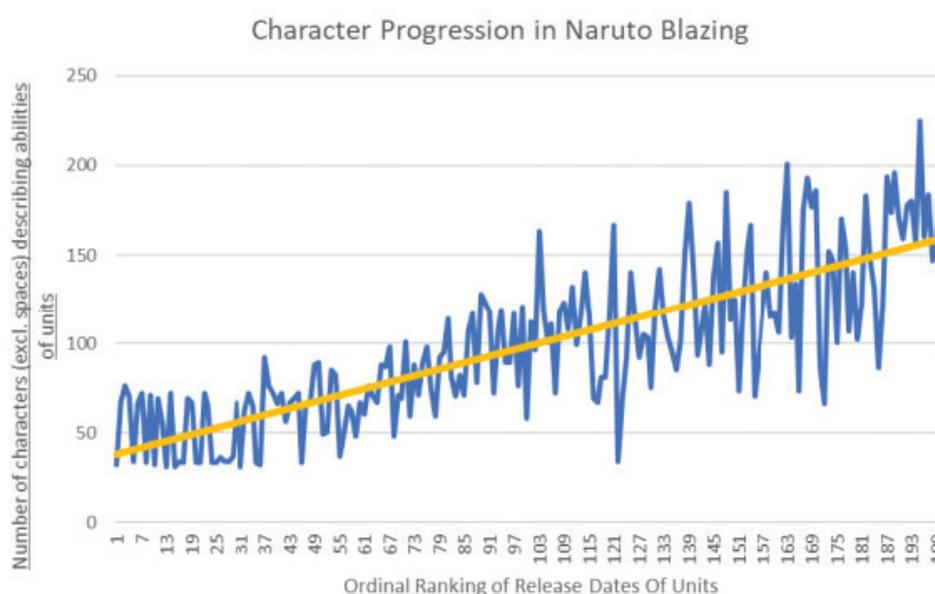


Figure 6: Illustrating the LOLLO measure for all 201 SSR units in the game. After measuring each description, I plotted them in a graph of characters (letters and spaces) against ordinal ranking with respect to release date. The orange line shows the trend line of appreciation.



Consequently, in gacha games, players pay hundreds of pounds just for a **chance** to pull a character which will only depreciate as new and better ones get released for the same effective cost. In fact, according to our LOLLO measure its only a matter of 5 weeks (on average) before the character, for which you payed hundreds for will be outclassed. (Based on how long it took for a character with a longer description to come out)

Competitive advantage:

The only significant benefit of spending to acquire a character, is the competitive advantage that getting that character sooner gives. When a new strong character comes out, immediately obtaining him and utilising him gives that player an advantage over others who have not got him yet and thus are now relatively weaker. Each addition of a new strong character to these game disturbs the previous power balance such that a player who does not have the new character, even if previously being one of the top players, no longer maintains that status. In fact, looking at the PvP (player vs player) tournaments for Naruto Blazing following the release of a new ground-breaking unit, the new unit is on average in 9 of the top ten teams. This illustrates how immediately acquiring the new character gives one a large competitive advantage in such intense multiplayer games.

IMPLICATIONS FOR FREE-TO-PLAY PLAYERS :

What does this mean for free-to-play players? Accounting for all the possible ways a free-to-play player can farm diamonds (in Grand Cross 7DS), the maximum amount he can possibly muster in a week is a mere 60 diamonds. This is only 1/10 of the amount needed to be expected to pull the weekly character and requires a consistent gameplay of 3 hours/week. By deliberately employing low rates and simultaneously restricting weekly diamond outflow, new characters are intentionally placed out of the reach of free-to-play hands 9 times out of 10.

As a result, it is not surprising that the majority, if not all of the competing players in the games' respective tournaments are pay-to-play. It is not possible for free-to-play players to fund the summons needed to support a competitive place in multiplayer tournaments such as those common in gacha games.

If free-to-play players want to be truly successful in a gacha game the best option would be to delay their consumption, save up their in-game currency and spend them on special event banners where the majority of ground-breaking characters are released (with the same drop rate and price of summoning, and thus the same effective cost). The characters released in special event banners (such as anniversary banners) tend to remain useful for a much longer period (10 weeks according to LOLLO) than what would be the case for normal banner units. These special event characters have a head start (in terms of ability) over the others that helps delay the devaluative effects that arise over time as newer and stronger characters are released for the same cost.

Why do players not defer their consumption, but spend their free currency on a regular weekly basis?

That said many people continue to spend on regular banners with lower quality characters. This seemingly irrational behaviour can be

explained in many different ways:

The first concerns the idea of information failure in that people are not fully aware of the implications of a 0.5% drop rate. In fact, after composing a survey in which 53 players of Grand Cross: 7DS were asked to estimate the expected diamonds needed to pull one copy of the featured unit, the average estimate was 31% lower than the actual value¹³. Most people, when estimating the diamonds needed, experience cognitive biases specifically the Availability Heuristic. Because players, in the game's communities, see posts concentrated with people pulling "so-and-so," they are led to believe that the chances of pulling "so-and-so" are higher than they actually are. This effect is also compounded with the optimism bias which suggests that people tend to overestimate the likelihood of good things. Both these effects result in an overestimation of one's chances, despite the rates being advertised on each banner.

Another reason why people summon regularly on these very expensive banners is because they manage to buy the in-game currency cheaply. With such a high cost for the purchase function, it is rather unsurprising that a black market for discounted in-game currency exists on the major social platforms despite the harsh penalties that warrant them. People desire in-game currency to summon for a character they like but are unable to do so because the diamonds are expensive. As such people, turn to third parties selling the in-demand currency at a lower price. This allows players to maintain a competitive advantage at a lower cost.

The final reason why players tend not to save but consume is because some games prevent it. By making the weekly diamond outflow progress-dependant as is the case in many gacha games, players trying to save are cut off from the weekly diamond supply. In order to collect diamonds to save, players must complete the harder missions each week, which in turn, requires the better characters that are regularly released. However, in order to get the better characters, one needs to summon regularly and so use up all their savings. In addition, many weekly missions have associated units whose stats are ameliorated making the mission much harder for those without the mission-specific unit. Therefore, both unit-specific missions and a fast-paced character development make saving and acquiring of new diamonds strictly independent activities.

CONCLUSION :

In conclusion, it is this "luck"-based gacha mechanism that makes these games so dangerous and potent. Having a purchase function (the acquisition of a desired character) without a specific price tag, allows these games to get away with, in many cases, extortionate costs like the one demonstrated above. Due to the variance of these rates, on one side of the spectrum people may get their desired character for free (within the 60 free weekly diamonds) but on the other side, players may spend over £1000 and still come out empty handed. The use of rates, instead of a fixed price, allows these games to hide the real (average) costs involved in the summoning process. By having to get the desired character through the gacha mechanism funded by purchased in-game currency, this indirect transaction system does not actually guarantee the player the character they paid for. These games are avoiding a quid-pro-quo payment exchange, justifying it through their use of "rates" and in turn funding a gambling-



like system for the character the player paid to get. It is this feature of coming out "empty-handed" and not guaranteeing players something to represent their purchase that makes games like these morally unjust and borderline scam-like. Instead they should be more revealing with respect to the implications of such a low drop rate to reduce the information failure and unawareness present in the majority of the games' communities.

It could be argued that such games do indeed, give players something to represent their purchase, through the other characters in the pool. Although not being what was originally desired, players may still benefit from the other SSR characters included in the banner, and thus benefit from spending money. That said, the majority of SSRs normally included in banners are often very old and therefore no longer as useful. Moreover, in some games there is no reward for obtaining the same character twice. This means for experienced players, who have acquired the majority of characters in the pool, the external (outside of getting the desired character) benefit from summoning is smaller.

Despite the harsh purchase function associated with the genre, a vast amount of people still play these games for various reasons. The first is because they ultimately enjoy the game. The majority of gacha games are, at heart, very fun to play. Gacha games often include very good mechanics and a unique gaming style that makes playing the game rather addictive. In fact, by looking at the specific reviews for "gameplay" on the Google Play Store, 20 randomly chosen gacha games all had ratings above 4 stars (for "gameplay"). This goes to show that the majority of gacha games feature enjoyable playing experiences, even if limited by in-app purchases.

A further reason people play such games regularly is because they enjoy the concept of a gacha-mechanism. For some, summoning characters from a pool is an exciting concept. It allows players to try their luck, and in the odd case, get the unit they desire at a discounted price, while also appreciating that sometimes they may get unlucky and come out with nothing. It is comparable to "responsible gamblers" who find the suspense and hype associated with luck-based pooling exhilarating. We can also go on to argue that the instances where players spend loads of money on a unit and come out with nothing are compensated by the welfare benefits they may gain later, upon acquiring a character within their first few summons.

Furthermore, not all gacha games come under the label of "scam-like," and indeed many who previously had, have now changed the game so it is more giving to players. *Naruto Blazing* is an example of such a game that has adapted and updated its content in accordance with the demands and requests of its player-base. Having previously featured a poor weekly diamond outflow with no guarantee of pulling the unit combined with low rates, the game has significantly improved. It has now implemented a guaranteed multi which gives the player the character for free after having spent 450 pearls or £210.96 on one banner. (Note "pearls" are a different currency from the "diamonds" in *Cross 7DS*). They have also increased the rates on banners drastically so that, 50% of the time, you need only spend half the pearls needed to reach the guaranteed step to get at least one copy of the featured unit. *Moreso* players can now obtain 55 pearls a week, as opposed to what had previously only been 27.

Ultimately, people play these games despite, in some cases, the extortionate prices, because they enjoy the game. F2P players can

have fun in these pay-to-win games if they accept that without paying they can not expect to get very far in the game's multiplayer element. Players only pay, typically from a competitive viewpoint, to gain the newest character which is often needed to maintain such a competitive foothold in the game.

'SCAM 2': "MULTIS" AND THEIR UNDERLYING PURPOSE

In this section we will see how "multis" are a more dangerous style of summoning compared to "singles" and how game developers often frame (and thus overexaggerate) the "multi-summon promotion" to get people to summon that way.

THE EXISTENCE OF MULTIS IN GACHA GAMES AS AN OPTION OF SUMMONING:

As explained previously, a 'multi' is, in most cases, where a player summons for 10 units in one go. Since each summon in a 'multi' is independent of one another, a multi can be modelled as 10 singles. The rates, if there was no incentive-system in play, would be the same for 10 singles as for 1 multi. However, in all Gacha games there is always an added bonus for "multis" that encourages players to choose that option of summoning. The very existence of an incentive system is an example of a ploy in play to make players spend more diamonds. By encouraging players to summon via multis, they lose their diamonds much faster and more easily, indirectly influencing them to purchase more diamonds when a new banner comes out for which they have nothing to spend.

HOW "MULTIS" ARE MORE DANGEROUS THAN "SINGLES"

When summoning a player is more likely to go overboard and spend more in-game currency, if summoning by multi's than he/she is by singles. This is due to the following reasons:

Firstly, each individual 'single' has lower rates (for a desired unit) than each individual 'multi'. Therefore, people have low expectations when entering a single. On the other hand, people expect much more from a 'multi', given that it is equivalent to (or because of the promotion, better than) 10 singles, and so their perceived gain from an incremental 'multi' is much higher than from an additional 'single'. Crudely put, people will be more encouraged to try their luck on an additional multi than on an additional single.

Moreover, it takes barely any time to buy one multi as opposed to 10 singles and so the period of deliberation or "pain of purchase" is reduced when one buys a multi. Clicking the button to buy one multi has the same outcome as clicking the button 10 times to buy a single. In the same way, the shorter transaction period also reduces the reluctance to summon from bad pulls. One will be more put off from summoning if he receives 10 Rs (rares) from 10 consecutive singles, than he would be if he got 10 Rs from one multi, as the "pain" is prolonged and spread out. In addition, because the results of a multi are compiled together, an element of decoupling is introduced. For example, the significance of a R would be downplayed if it was



received with an SSR in a multi, than if it was received separately via singles. Therefore, summoning by multis decreases the demotivation to summon from bad pulls.

Consequently, the likelihood of overspending is higher for multis than it is for singles. Not only that, but the cost of going overboard is much higher for multis too since they cost 10x as much as singles. If one were to buy one more single than they originally planned, the cost would only be 3 diamonds¹⁴. Yet, if one were to buy one more multi than they originally planned, the cost would be 30 diamonds (impulsively clicking to buy a multi costs ten times as much as impulsively clicking to buy a single). On the other hand, it is similarly easier to save diamonds on 'singles' than it is for 'multis', as multis are in denominations of 10 as opposed to 'singles' and thus, one has to spend 30 diamonds on what would be the determining trial, but only 3 if it were a single, (i.e. with singles you can stop directly after the unit has been acquired, but with multis you must follow through with, in the worst case, the 9 following units.) Combine both the added cost and likelihood of overspending and we see that multis are a much more dangerous style of summoning compared to singles. Therefore, having a system (in the first place) encouraging players to summon via multis would indirectly increase the amount of diamonds purchased as players find themselves without their free hard-earned diamonds rather quickly.

Hence whilst the incentive-system (the added promotion) for multis does make the rates somewhat better than singles, it leads to overconsumption of diamonds (especially of free hard earned diamonds) than what would have been the case if the player had summoned by "singles."

FRAMING OF THE PROMOTION/ INCENTIVE SYSTEM:

In most cases, the incentive system itself is also a product of behavioral tricks causing players to overestimate by how much a multi is better than a single. Consider the multi-summon promotion in *Naruto Blazing*: "At least one SR or higher guaranteed." When players encounter this promotion they would be more inclined to summon via a multi due to the inclusion of the guaranteed unit, which could either be an SR or an SSR (the more desired option). However, such a promotion can be carried out in different ways, some of which fulfill the promotion yet have little added benefit to the players.

In order to compare the different possible promotions, we will be analyzing the effect each scenario/promotion has on the random variable: "expected number of SSRs per multi summon," using the distribution for "singles" present in the game: R(67%), SR(30%) and SSR(3%). (i.e. model the multi as 10 singles and factor in the promotion, which is, indeed, what a multi is).

Originally with no added promotion (our base case) the expected number of SSR's per multi summon is $10 \times 0.03 = 0.3$ SSRs per multi. (This is the same as doing 10 'singles')

Now consider the first and most beneficial scenario (Scenario A): 1 character is pulled from an SR/SSR pool, and the rest are from the pool with the given distribution above. The chance of pulling an SSR from the one summon from the SSR/SR pool is $0.03 / (0.33) = 0.091$, and the chance of pulling an SSR from the 9 summons in the

larger pool is $0.03 \times 9 = 0.27$. By adding them together we see that the expected number of SSRs' per multi increases by 20.3% to 0.361 SSRs per multi. This gives the players a very large increase in rates (for an SSR), and relies on the assumption that the distribution of SSRs and SRs in the SSR/SR pool is proportional to that of the original pool which may not be the case. In fact the SR/SSR pool may have its own unique distribution for which the chance to pull an SSR is dampened.

Our second scenario (Scenario B) involves removing the possibility of getting all 10 units as rares from the sample space, by re-summoning if 10 Rs are generated. This will, in turn, ensure that the player gets at least one SR, or SSR. Since the chance of getting all Rares is $(0.67)^{10} = 0.0182$, by reducing our sample space we see that the expected number of SSR's per multi jumps to $0.3 / (1 - 0.0182) = 0.306$, or grows by 1.86%. This fulfills the promotion but results in a sharply lowered added benefit for the players compared to scenario 1. Even so, the developers could do better:

In our final scenario (Scenario C), 9 characters are pulled from a regular pool. If all 9 are R, the 10th unit is pulled from an SR/SSR pool. The probability of getting 9 Rares from 9 consecutive summons is $(0.67)^9 = 0.0272$. This means that the expected number of SSRs per multi, according to this scenario, is:

$$\begin{aligned} &= P(\text{Not getting 9 R's}) \times (\text{Expected number of SSR's per 10 summons}) \\ &+ P(\text{Getting 9 R's}) \times [(\text{Expected number of SSRs per 9 summons}) + \\ &P(\text{Getting an SSR from the SR/SSR pool})]. \\ &= (1 - 0.0272)(0.3) + (0.0272)(0.17 + (0.03/0.33)) = 0.302 \text{ (3 s.f.)} \end{aligned}$$

This is a mere 0.552% increase in the expected number of SSRs compared to our base, non-promotion case. Therefore, whilst the promotion may look very good, somewhat like scenario 1, in reality it could be very minimal, more like scenario 3. This is an example of framing, whereby framing a statement or offering it in a different way generates a new response, by changing the comparison set it is viewed in. In our case, the promotion "get an SR or higher guaranteed," sounds better and is the positive form of "guaranteed to not get all Rares," which is essentially what the promotion is getting at. The latter statement is the same as the former but shows clearly that the only case in which a multi is better than a single, is when you get 10 consecutive singles as Rs which is quite rare.

Of course, with the aim of generating as much money as possible, the developers would choose the positive formulation of the statement and an algorithm (or scenario) which minimizes the rates of pulling an SSR, lulling players into overestimating their chances when summoning via 'multis.' This would, in turn, encourage them to summon more dangerously (through 'multis' instead of 'singles') and buy more diamonds when they have churned through all the diamonds they had and still not pulled what they originally desired (as a result of the low rates).

However you may be thinking that there are a lot of uncertainties in this analysis, which I agree with. It may be that scenario 1 is the actual system adopted by the game as opposed to the third, rate-minimizing, option¹⁵. Since we are not the game developers it is not possible to see which scenario is in play or even whether it is one of the three demonstrated above at all. For example, the distribution used to make our base case (of 0.3 SSRs per multi) was based on the distribution for 'singles', and so 'multis' may have their own unique



distribution (by distribution I am referring to the percentage drop rates for Rs, SRs, and SSRs). Similarly, as mentioned previously, we also assumed that the SR/SSR pool rates were proportional to the original distribution which may not be the case. Given that our analysis was solely based on assumptions, this begs the question, what can it possibly prove? Well, this analysis does serve to prove one point: that the promotion may not be as good as it seems from first impressions. Framing is a very powerful behavioural tool that can manipulate the outcome of our choices solely based on how the same information is presented. Indeed, although guaranteeing an SR or higher, Bandai may only have increased the rates by half a percent compared to 10 singles, falsely motivating players to quickly spend all their free hard-earned diamonds in the process.

Having said that, there is a statistical tool that we could use to see which of our proposed scenarios the actual distribution of a 'multi' favors. This would allow us to get at Bandai's true motive: money or sincerity. This tool is called a "Goodness of Fit Test," and we will be using it hand-in-hand with a "Chi-Squared Test," to evaluate how closely our model fits the actual distribution. By examining multis from the game via online summoning videos posted by relevant content creators we will be able to compare the actual numbers of SSR's pulled to what would be expected given our model was true, or near the truth. There are several problems with such an approach, however. Firstly, content creators tend not to post the full story of their summons. They tend to summon off-camera and in some cases only post the highlights instead of the whole summoning process. This problem can be avoided by watching posted live streams where all summoning was done on camera. Furthermore on the edited videos we can choose to analyze only a handful of summons at random intervals throughout the video, which should reduce any bias. The second problem concerns updates and uncertain timing. The 'single' summon distribution used to make our base non-promotion case, was sourced from 2017 and the rates have since changed in proceeding updates (June 2020). Consequently, we will only be able to refer to videos in the year the rates were sourced from, (2017)

After compiling enough data from appropriate summoning videos, I recorded 200 (20 multi) summons and listed whether they were SSRS, or not. Then underneath the observed pulls I calculated what would be expected given each of the scenarios were true:

	Number/Frequency of SSRs pulled	Number/Frequency of non SSRs pulled
Observed pulls (O_i)	54	146
Expected pulls given Scenario A was true (E_{iA})	72.2	127.8
Expected pulls given Scenario B was true (E_{iB})	61.2	138.8
Expected pulls given Scenario C was true (E_{iC})	60.4	139.6

To compare which model is closest to the actual distribution (the observed pulls) we need to conduct a Goodness of Fit test (GoF). A GoF test measures how well an observed frequency distribution fits to a known distribution.

To conduct a Goodness of Fit test we calculate X^2 from the following formula:

$$X^2 = \sum_{i=1}^n \frac{(O_i - E_i)^2}{E_i}$$

where O_i is the observed frequency and E_i is the expected frequency asserted by the null hypothesis (which in our case is that the respective scenario is true)

After rearranging, a simpler equation for X^2 can be found:

$$X^2 = \sum \frac{(O_i - E_i)^2}{E_i} = \sum \frac{O_i^2 - 2O_iE_i + E_i^2}{E_i}$$

$$X^2 = \sum \frac{O_i^2}{E_i} - \sum \frac{2O_iE_i}{E_i} + \sum \frac{E_i^2}{E_i}$$

$$X^2 = \sum \frac{O_i^2}{E_i} - \sum 2O_i + \sum E_i$$

$$X^2 = \sum \frac{O_i^2}{E_i} - \sum O_i$$

$$X^2 = \sum \frac{O_i^2}{E_i} - N$$

$\sum E$ and $\sum O$ are both equal to N as they represent the total number of trials and or observations

With this simpler equation for X^2 we can now find the Goodness of Fit results for our three scenarios.

$$\text{Scenario A: } X_A^2 = \frac{54^2}{72.2} + \frac{146^2}{127.8} - 200 = 7.18 \text{ (3.s.f)}$$

$$\text{Scenario B: } X_B^2 = \frac{54^2}{61.2} + \frac{146^2}{138.8} - 200 = 1.22 \text{ (3.s.f)}$$

$$\text{Scenario C: } X_C^2 = \frac{54^2}{60.4} + \frac{146^2}{139.6} - 200 = 0.972 \text{ (3.s.f)}$$

Given that the higher the value of X^2 the less similar the observed distribution is to the theoretical distribution, we can see from face value that Scenarios B and C are better models for the in-game multi rates than the more generous Scenario A.

However, since the sample is quite small at only 200 observations, natural variation has a larger effect on our Goodness of Fit test. In other words, we may have recorded unusually low data from our sample. Consequently, carrying out a hypothesis test (by means of a Chi-Squared Test) for scenario A will allow us to see how much the difference from the observed data can be justified by natural variation.

To complete a hypothesis test we have to formulate the null and the alternative hypotheses given by H_0 and H_1 respectively.

H_0 : Scenario A matches the in-game model for multis in Naruto Blazing

H_1 : Scenario A does not match the in-game model for multis in Naruto Blazing

Note that all hypothesis tests for GoF are always one-tailed as GoF tests are always positive. This means the critical region is always the set of values above the critical value.

The critical value for our test depends on both the number of degrees of freedom and the significance level at which we choose to conduct our hypothesis test. The number of degrees of freedom from our data is 1, because knowing the amount of SSR's pulled uniquely determines



the amount of SSR's not pulled as we have a constraint of 200 total observations. (If we pull x SSRs, we know we have pulled $200-x$ non SSRs. This data point is therefore no longer "free". It is dependant because we have a constraint.) Thus the constraint of 200 total observations takes up one of the two data points leaving only one data value not used up and free to vary (independent.)

For our hypothesis test we will choose a significance level of 1%.

This means the critical value for our test is thus $\chi^2_1(1\%) = 6.635$

The subscript "1" refers to the degrees of freedom, and the bracketed percentage references that this test is being measured at the 1% significance level.¹⁶ Note how it is no longer X^2 , but chi-squared because we are finding the critical value by referencing a member of the chi-squared family of distributions, with the same degrees of freedom and significance level as ours. (This is the chi-squared test)

Hence if the GoF test for Scenario A exceeds 6.635 we can conclude that it is in critical region and thus not a suitable model. Since $\chi^2_A = 7.18$ which is greater than 6.635, it is indeed in the critical region and so there is sufficient evidence at the 1% significance level to reject H_0 in favour of H_1 and conclude that Scenario A is not a suitable model even with natural variation accounted for.

I chose a very low significance level because it minimised Type 1 error. Type 1 error is the percentage chance of incorrectly rejecting H_0 . Since we want to be as accurate as possible when dismissing scenario A as the potential in-game model, choosing a 1% significance level means that there will only be a 1% chance that the GoF test is greater than 6.635 due to natural variation. This in turn, tells us that there is a 1% chance our conclusion is wrong and scenario A is indeed the in-game model. However, because this is very small we can be confident in rejecting Scenario A and concluding that Bandai (the developers of Naruto Blazing) have opted for a more hard-giving multi summon promotion, framing it in such a way that it seems better than it is, lulling players into spending their hard-earned in-game currency quickly.

When carrying out the hypothesis test for both Scenarios B and C, the hypotheses would again be:

H_0 : Scenario B/C matches the in-game model for multis in Naruto Blazing

H_1 : Scenario B/C does not match the in-game model for multis in Naruto Blazing

(Depending on which scenario we are testing)

However, because their GoF tests are very close to 0, (1.22 and 0.972 respectively), we pretty much know already that we will accept H_0 as it is less than 6.635 and so not in the critical region (that is if we used the same significance level as done with scenario A)¹⁷. So instead we want to minimise Type 2 error. Type 2 error is the percent chance that you accept H_0 but H_0 is actually false. In our case, this means the percent chance that Scenario B/C is not the model in the game and that the GoF test chose not to fall in the critical region by natural variation (i.e. the data was unnaturally low enough to not satisfy the critical region for our test.) Since Scenarios B and C are very similar to the in-game distribution (according to the GoF tests) we want to choose a larger significance level. This means it is easier for our chi-squared test to fall in the critical region (as it is now larger) and

thus easier to reject H_0 . This reduces Type 2 error by making it easier for what may have been a different distribution or natural variation, that had falsely suggested a close relationship between the in-game model and B/C, to fall in the critical region and now be accounted for.

Whilst with Type 1 errors we can find the percent error as it was simply the significance level, Type 2 errors usually can't be quantified because to quantify them we need to know the actual distribution present in the game. From then, we calculate the probability of that distribution not falling in the critical region. Since we do not have that information, for the sake of simplicity,¹⁸ we will choose a significance level of 10%, which should in theory, minimise Type 2 error drastically. Furthermore, due to the small size of our sample, it will be difficult to distinguish whether the in-game model favours Scenario B or C, because they only differ by 0.8 in expected number of SSRs pulled. This means both scenarios will have the same results for our chi-squared tests, and so for brevity we will only look at scenario B, because if scenario B succeeds, scenario C, which is closer to the observed pulls, will also succeed.

The hypothesis test for scenario B is as follows:

H_0 : Scenario B matches the in-game model for multis in Naruto Blazing

H_1 : Scenario B does not match the in-game model for multis in Naruto Blazing

Since we have 1 degree of freedom as we are referencing the same data used in the hypothesis test for Scenario A and we are using a significance level of 10%, the critical region is as follows:

$$\chi^2_1(10\%)=2.705$$

Because $\chi^2_B = 1.22$ which is less than 2.705, it does not fall in the critical region. Therefore there is insufficient evidence at the 10% significance level to reject H_0 and so we can conclude that $X_{B/C}$ is likely to be the in-game model.

These hypothesis tests ultimately shed light on our original statement: that promotions, particularly good ones are not always as they seem. In Naruto Blazing, we can see that their main aim is Money not Sincerity, because although guaranteeing an SR/SSR they have chosen to increase the expected number of SSRs per multi by only 1.86 or 0.552% or similar, despite the easiest way to carry out their statement (Scenario A) involving a 20.3% increase in rates. By deploying a statement with ambiguity and a false sense of hope in their multi-summon promotions, many gacha games are lulling players into going down the dangerous route of summoning, indirectly nudging them to buy more diamonds/pearls.

EVALUATION:

In evaluation, there are flaws in the argument for multis being a more dangerous route of summoning. Firstly this argument does not apply to gacha games for which the multi-summon promotion is good enough to warrant the more dangerous route. For example, in Grand Cross 7DS, whilst a multi costs the same as 10 'singles,' a multi gives the player 11 characters instead, effectively giving them one free. This already gives multis a 10% increase in the expected number of SSRs compared to the equivalently priced 10 singles. Such a large increase



in rates outweighs the potential hazard of overspending that comes from summoning by multis. In addition, whilst argued previously that “singles” are a better way of saving over multis given that you can stop directly after the determining trial, (whereas with multis you have to, in the worst case, follow through with the 9 other summons), this point is made redundant if the multi-summon promotion is good enough to reduce the expected number of summons by 9 or more. In fact, in the case of Grand Cross 7DS, not summoning by multis poses a large opportunity cost to the consumer as they are not maximizing the value they could have bought when summoning through singles. For each multi, not bought the consumer effectively loses one summon.

This leads on to our second point, in that players should instead summon by multis but in doing so, budget their spending. If players adhere to a strict budget, then they can make fruit of the increased rates associated with multis whilst also not overspending, leaving more in-game currency to be spent on an upcoming banner. That said, as we will find in the consequent section; budgeting one’s spending is much harder than it seems, especially in gacha games with “pity systems” incorporated in.

It this “pity-system” and reduced pain of purchase associated with multis combined that leads to heightened overspending.

‘SCAM 3’: PITY SYSTEMS

In this section we will be looking at a so-called “Pity-system” common in the majority of Gacha games. Whilst often disguised as a sympathetic reward system it, in most cases, acts as a carrot on a stick model incentivizing players to spend just that little bit more to a seemingly “golden” reward.

THE EFFECTS OF THE PITY SYSTEM:

The majority of gacha games feature these pity systems in their multis, which can be seen as a method to lay people off of their original budgets. A pity-system is an in-game system that compensates players with bad-luck, who have spent a lot of in-game currency to no avail.



Figure 7: Shows the pity bar, (under “Draw Bonus”) which fills up 20% after every shaft.

In Grand Cross 7DS, for example, if you get 5 shaft multis (which needn’t be consecutive), your next multi will include a guaranteed SSR. These pity-systems, similar to the multi-summon promotions, have some benefits but tend to only be exclusive to pay-to-play players.

Before we digest the statistics behind pity-systems and to what effect they increase rates to pull desired characters, we need remember to account for the multi-summon promotion in Grand Cross 7DS

Since the promotion is the inclusion of a free unit, when we model the multis as binomial distributions with n trials and probability of success, p , we must remember that for multis the number of trials $(n)=11$, whereas for independent singles, $n=10$.

That covered, we can move on to analyzing the effect of the pity system in Grand Cross 7DS. We must remember that the pity system only comes into effect after 5 shaft multis, or 5 multis in which no SSR’s have appeared. After every summon a pity bar is shown which, after each shaft, fills up. Once full, after 5 shaft multis, an SSR is guaranteed on the next multi.

Hence, we can calculate after how many multis, on average, the pity system comes into use.

Because we are concerned with the amount of SSRs per multi and not the amount of desired units, our binomial distribution has changed to:

*Let X be the number of SSRs per multi
such that $X \sim B(11, 0.03)$*

Our probability parameter has changed to 3%, as that is the drop rate for SSRs. Thus the probability of being shafted is:

$$P(X=0) = 0.97^{11} = 0.715 \text{ (3.s.f)}$$

Therefore, the number of trials needed to get 5 shafts is:

$$\frac{5}{0.7153} = 6.99006 \dots \text{So by the 7th multi you are expected your 5th shaft}^{19}$$

As a result of the pity system the multi after it, expected to be your 8th, will feature a guaranteed SSR. We must treat this multi differently as the rates will be different from an ordinary 11-character summon. The probability of pulling at least one desired (banner featured) unit in this multi is the probability that we pull at least one copy in the 10-ordinary summons (called Event Y) plus the probability that we pull him from the one summon from the SSR pool, (which is essentially what the guaranteed SSR is) (called Event Z).

The probability of Event Y happening is:

*Let X be the number of desired units per 10 summons such that:
 $X \sim B(10, 0.005)$*

$$P(X \geq 1) = 1 - P(X=0) = 0.0489 \text{ (3.s.f)}$$

And the probability of Event Z happening is:

$$\frac{P(\text{pulling desired unit})}{P(\text{pulling an SSR})} = \frac{0.5}{3} = \frac{1}{6} \text{ or } 0.167 \text{ (3.s.f)}$$

Hence the total probability of pulling at least one copy of the desired unit on this multi is $0.167 + 0.0489 = 0.216$ (3sf)

This is just over 4 times the rate for regular multis.



Therefore, if we imagine the 8 multis as a **cycle**, the probability of pulling at least one copy of the desired unit in this cycle is:

$$0.216 + P(\text{Pulling at least one copy in each of the 7 multis}) = 0.216 + 0.376 \text{ (3.s.f.)} = 0.591.$$

Therefore, using the mean of a geometric distribution with parameter 0.591, we see that on your 1.69th cycle you are expected to pull at least one copy of your desired unit. Be that as it may, with both 1.69 not being a whole number and our cycle consisting of 8 multis, which is a large denomination, it is difficult to pinpoint on which specific summon you are expected to pull at least one copy of the desired unit. However, since we know that the expected multi lies 69.2% along our second cycle we can use linear interpolation to determine the expected value of multis needed. Seeing that the 8th multi (or the pity-multi) in our cycle is on par with 4 ordinary 11-character multis we will have to adjust our interpolation proportionally. In other words, we cannot interpolate on a scale with 8 equal partitions, as the 8th partition or multi has a much larger drop rate for our desired unit than the other 7. By using the probability value of 0.591 as being 100% along the cycle, each multi, should, with their respective probability values be proportionally represented. This means being 69.2% along our cycle is to be at the probability value of $0.692 \times 0.591 = 0.409$ (3sf). So, the multi in the cycle that gets our cumulative probability above 0.409 will be the determining multi (to be expected to get the desired unit.) The probability of pulling at least one copy of the desired unit in the first seven multis is $7 \times (1 - 0.995^{11}) = 0.3755$ (4.s.f). Since 0.409 is greater than 0.3755, the expected multi is the final one in our cycle. This means, on average, you need to complete 2 cycles or summon 16 times to be expected to pull the desired character at least once. Therefore, as a result of a pity system one only saves 3 multis or 16% of their diamonds as opposed to a scenario without the pity. As enticing as it may seem, the pity system is, however, yet another ploy in play to make players purchase diamonds. The explanation can be derived from the nature of the pity system itself:

THE PITY SYSTEM AS YET ANOTHER PLOY:

Firstly, as mentioned previously the benefits of this system are strictly pay-to-play exclusive. In order to reap the rewards of the pity-system a player must have been shafted 5 times. This means one needs minimum 180 diamonds, (for 6 multis, assuming the first 5 were shafts), or the expected 240. That said, a free-to-play player can only amass 180 diamonds after 3 weeks given the restriction in diamond outflow. Therefore the pity system, being conveniently placed out of the reach of free-to-play hands, can encourage the purchasing of diamonds to close that gap and make fruit of the heightened drop rate for the desired character that would otherwise be unattainable. The drop rates for the pity system are deliberately large in comparison to ordinary multis in order to motivate players to pay to reach it, yet simultaneously low in absolute terms such that it fails 4 out of 5 times, welcoming players to try their luck again.(i.e. by going another cycle)

Most importantly, the pity system serves as a quintessential example of the sunk cost fallacy in play. The sunk cost fallacy applies to the continuation of a behavior or endeavor only as a result of previously invested resources. Frankly put, it is a scenario in which a person

follows through with an action in the hopes of recovering an already lost value. Perfectly contextualized by Shakespeare, Macbeth says "I am in blood, stepped in so far that should I wade no more, returning were as tedious as going o'er." It occurs when deliberating on whether to continue and risk further losses or stop and forgo your losses. In our game, the sunk cost is invested diamonds on a banner which have not pulled the desired unit. Players, in accordance with the fallacy, and in attempts to make the most of the already lost diamonds choose to spend real money to summon more and fill the pity bar, which had been partially filled by the already spent diamonds. As such, people are motivated by the false thought of redeeming the value of the diamonds lost, to purchase more diamonds and summon on the pity which has a higher chance of fulfilling their original goal. Because each cycle ends with the pity multi, which is on par with 4 multis, people may view an already semi-full pity-bar and feel the need to fill it by summoning more, given it would be a waste of "invested resources" when the pity refreshes. To echo one's internal reasoning: "I have gone this far, I may as well follow through." Hence refreshing the pity every week for each new banner puts pressure on players not to let their progress to a reward go to waste. Hence, the pity gives players a reason to summon further when there would otherwise not be.

In addition, by pushing the pity-system far from reach and showing progress towards the pity system after each summon as shown in the picture below, players count their multis in terms of how close they are to the pity rather than in absolute terms. This can lead to players losing count of how many multis they have spent, as they focus solely on reaching the pity.

Consequently, the pity-system ultimately serves as a reason to continue summoning rather than a benefit whilst summoning. By having it only activate after 5 shafts and not after a specific amount of summons there is no knowing for certain when a player will achieve the pity. Such uncertainty can lead to players underestimating how many multis they need to commit to complete a cycle, leaving them to buy more diamonds when they come to the realization that the multis bought are not enough and will go to waste if more aren't bought to fill the pity (This in turn, makes budgeting one's spending very difficult). In conclusion, the pity system is merely a motivation to summon, playing on our inherent overweighting of sunken costs. It uses short time spans and constant reminders after every summon to further the irrational decisions telling us to continue. Therefore, the pity multi (with its large rates) acts an anchor or a carrot at the end of a stick, telling us to stop at the end of a cycle than in the middle of one, making us spend diamonds to complete the partial cycle we would have otherwise finished on.

CONCLUSION

In conclusion, from our above analysis we can see how the gacha mechanism, associated with extremely low rates and its respective pity system, is extremely costly and hence pay-to-play exclusive.

This ultimately begs the question, "is it really a scam, then?" According to the Cambridge English Dictionary a scam is "an illegal plan for making money, especially one that involves tricking people." We can safely say that "scam" is perhaps too strong a word as the gacha mechanism is not illegal. The latter part of the definition, however,



could be argued to be applicable. One may claim gacha game developers are tricking people through the framing of their multi-summon promotion, their purposefully designed pity-systems and incredulously low rates. However, to trick someone implies to cheat someone and that is not what gacha games are doing. Gacha games are simply bending the truth, hiding away the ugly side of the facts under an appealing guise for the players. They are still advertising their rates, pity-system and multis but it is the players not fully realising the cost in their cost-benefit analyses, that is the problem. Gacha games do display the true chances for pulling specific units (for not doing so would be illegal) but they themselves along with external contribution influence the player to overestimate those chances. The individual, always has a choice when it comes to purchases, but Bandai and other gacha developers influence that choice by downplaying the cost of the item. This is often through how the game is presented which feeds subliminal messages to the consumer as they navigate through the games' menus (this is also aided by the seamless transaction system mentioned in the introduction).

This is not to say, however, that gacha is unlike gambling. Fundamentally the gacha mechanism has incorporated a sense of gambling into purchases. It has the potential to make purchases redundant (i.e losses) if the bought in-game currency fails to achieve what was first aimed for by it. Perhaps it is the sense of no or minimal compensatory benefits and uncertainty as to when a player will acquire the new unit (to acquire a unit) that is the most gambling-like aspect of the game. Despite the luck and unluckiness associated with these summons, players will still, on average, pay large sums for highly illiquid assets which can't be traded on and only depreciate as the game progresses. Indeed these purchases will bring utility to the consumer, but is this the maximum utility that could have been bought? One needs to distinguish whether paying this amount of money for a virtual in-game character is the result of maximising utility or an addiction or likewise obsession to collect all the characters/units that, in turn results in a lower indifference curve being selected and thus lower achieved utility.

Ultimately it is unfair to make generalisations to the genre. Indeed, some games do exhibit the "ploys" mentioned in this essay, whilst others don't. We can't forget, these games are providing a service in the form of their games which are generally of high quality, for free. Their payment system, therefore, being heavy in-app purchases allows these games to keep the barrier to download virtually non-existent. Being free-to-play does not mean the game is necessarily unplayable, but it just slows down or caps progress and you lose out on events/activities that pay-to-play players would otherwise receive. Such games need to satisfy the free-to-play playerbase as it makes up a large proportion of players playing these games. If free-to-play players did not play these games, then pay-to-play players would not pay to maintain a competitive advantage as there would not much competition left to gain a foothold on.

These games are very good at targeting or even exploiting consumer weaknesses at computation. Playing on the sunk cost fallacy, their use of framing and heuristics (due to external contribution and the presentation of these games) allows them to make a lot of money as people spend more money than they would rationally adhere to. Indeed, after asking many regular buyers about their first purchase, the majority of them said it ended in "regret", although that did not stop

them buying more.

The best solution to this would be avoiding being overly attached to games like these, or to sunken costs. Being able to drop the game easily and substitute to other forms of entertainment will allow consumers to maximise utility especially when they realise that they no longer enjoy the game, and are solely playing, on the basis of their invested resources (to not let their account on which thousands of pounds was spent go to waste/depreciate). These games feed on the addiction of players with little self-control. Such players are caught in a weekly cycle, paying for a new character which is always going to be better than the last. Gacha games' exploitation of these consumer weaknesses, whilst legal, are morally unjust as it does not give the consumer the right frame of mind to make rigorous and accurate cost/benefit analyses when making a purchase. This leads to an inefficient allocation of resources in that other games which may provide a better service and better utility for a lower cost are not realised.

That said, such exploits of consumer weaknesses leading to irrational decisions in favour of the producer is common in our modern world. However, it is the fact that the gacha genre is taking advantage of addictions and even supplies them with the constant release of newer better units each week for the same absurd price is what distinguishes these games from the rest of the world.

Unfortunately, however, these "tricks" are unlikely to be changed. When brought up, gacha games will always argue their side of the story; that the pity-system sympathises with players, that the multis act as a convenience and that the multi-summon promotion is just stating the truth. In fact, in the future we can expect to see more instances of the "gacha-mechanism" as other companies take aboard this successful approach, and the existing companies grow larger and expand their operations testing the boundary even further into "scam-like" territory.



Creating colour: The chemistry of dyes

Alex Thow

SECTION 1 INTRODUCTION

To truly understand the chemistry of dyes we first must consider their colour. Colour has fascinated humans for thousands of years, from Aristotle believing it was sent from heaven, to Newton separating light into its colours with a prism. Our curiosity with colour comes from a young age, asking our parents why the grass is green and the sky blue.

To start this exploration of colour we will look at some basic quantum mechanics to study the behaviour of light and particles. These ideas can be applied to give an accurate picture of how electrons behave in atoms and molecules. From this, a description of bonding and delocalisation in organic molecules can be built up and used to explain how certain molecules can absorb visible light, giving them colour.

The focus of the text will then shift to a more general look at dyes. A glance over the importance of dyes in human history and their development will be covered before moving into the organic composition of dyes. We will then look at the structure of some materials and how they can be dyed and bleached. To finish off our discussions we will consider some specific examples that display how an understanding of the chemistry of dyes can explain different physical and biological phenomena.

SECTION 2 QUANTUM MECHANICS

2.1 A BRIEF HISTORY

2.1.1 Blackbody Radiation

In 1900, Max Planck began a scientific revolution. At the time there was a problem, known as the ultraviolet catastrophe, with something called blackbody radiation. This is the radiation of electromagnetic waves from an object that absorbs and emits all frequencies of light. A law can be derived from classical physics, Rayleigh-Jeans' law, that links the intensity, B , of radiation to the frequency, ν .

$$B(\nu) = \frac{2\nu^2 k_b T}{c^2}$$

In this equation, k_b is the Boltzmann constant, c the speed of light in a vacuum and T the temperature of the black body. This law worked for low frequencies but as the frequency increased, it diverged from the observed spectrum. What Planck did was to assume that the emissions of radiation did not take a continuous range of energies but had discrete energies proportional to integer multiples of their frequency.

$$E = n h \nu, \quad n = 1, 2, 3, \dots$$

He called the constant of proportionality Planck's constant, h , and used his assumption to create a new law for blackbody radiation, Planck's law.

$$B(\nu) = \frac{2h\nu^3}{c^2 \left(e^{\frac{h\nu}{k_b T}} - 1 \right)}$$

Using this equation and experimental data, he calculated the value of h to be $6.626 \times 10^{-34} \text{ J s}$. Planck's law fit the observed spectrum perfectly, but he had no idea why this was the case.

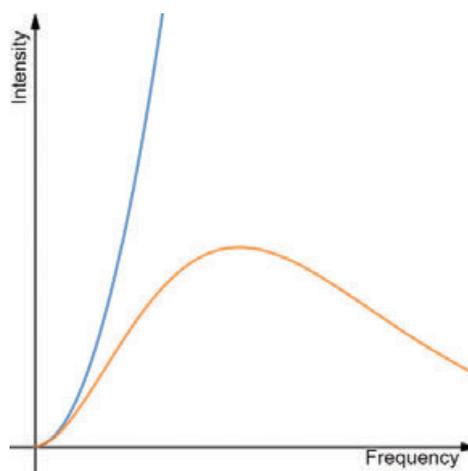


Figure 1 - Graph showing blackbody radiation. In blue is Rayleigh-Jeans law and in orange, Planck's law.

2.1.2 The Photoelectric Effect

Within the year 1905, Albert Einstein published four groundbreaking papers and so this year is called Einstein's 'Annus Mirabilis'. The first of these, for which he was awarded the Nobel prize in 1921, explained the photoelectric effect. This is a phenomenon in which light above a certain frequency, when shone onto the surface of a metal, can kick out electrons. The higher the frequency, the faster these electrons travel. No classical explanation had been found since the effect's discovery in 1887.

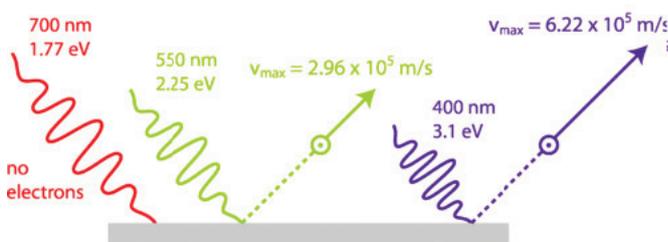


Figure 2 - Diagram showing the photoelectric effect.

Einstein deduced that every observation could be explained by assuming that light was made up of particles, photons, with energy directly proportional to their frequency.

$$E = h\nu$$



The constant of proportionality is Planck's constant, h . Einstein reasoned that a photon could transfer its energy, $h\nu$, to an electron. If the photon had enough energy, it could kick the electron out of the metal. Any extra energy that the photon had would become the kinetic energy of the electron, E_k .

$$E_k = h\nu - \phi$$

The letter ϕ denotes the work function and is the minimum energy required to kick the electron out of the metal. The assumption that light was made of particles was a radical one, so was not widely accepted until 1916, when experimental results confirmed Einstein's theory.

2.2 THE SCHRÖDINGER EQUATION

2.2.1 An Introduction

Over the years, quantum theory developed as more rigorous mathematical descriptions were formulated. Perhaps the most well-known is the Schrödinger equation, which describes something called the wavefunction of a system, denoted by the Greek letter, ψ . The first postulate of quantum mechanics is that the state of a quantum system is completely specified by the wavefunction. A classical parallel would be a set containing the positions and momenta of all the particles in a system. Schrödinger's equation does have time-dependence, but for the systems we will be covering, a time-independent equation can be used.

$$\hat{H}\psi = E\psi$$

2.2.2 Operators, Eigenfunctions and Eigenvalues

The first term of the time-independent Schrödinger equation is \hat{H} . The hat symbolises that this is an operator, which is a mathematical object that turns a function into another function. They can take a wide variety of forms. For example, the operator $\hat{A}=x$ simply multiplies the original function by x , whereas the operator $\hat{B}=\frac{d}{dx}$ differentiates it with respect to x .

$$\hat{A}\sin(kx) = x \times \sin(kx) = x\sin(kx)$$

$$\hat{B}\sin(kx) = \frac{d}{dx}\sin(kx) = k\cos(kx)$$

For a given operator, \hat{O} , if a function, $f(x)$, gives back the same function multiplied by a constant, λ , that function is called an eigenfunction of \hat{O} and λ is the corresponding eigenvalue.

$$\hat{O}f(x) = \lambda f(x)$$

2.2.3 Operators in Quantum Mechanics

The second postulate of quantum mechanics is that for every classical observable, there is a linear, Hermitian operator in quantum mechanics. We will not discuss here what it means for the operator to linear or Hermitian, but all the operators we will see obey both criteria. An example of the second postulate is that, corresponding to the classical observable of linear momentum along the x -axis, there is a quantum mechanical operator, \hat{p}_x .

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$$

Note that $i = \sqrt{-1}$, $\hbar = \frac{h}{2\pi}$ (the reduced Planck's constant) and $\frac{\partial}{\partial x}$ is the partial derivative with respect to x , meaning that any other variable is treated as a constant. A discussion of the origins of this operator is too in-depth for this text, but it can be taken as an axiom.

The operator in the Schrödinger equation, \hat{H} , is the Hamiltonian

operator. It is the operator corresponding classically to the total energy of a system. From classical mechanics, the total energy is the sum of the kinetic energy and potential energy.

$$\hat{H} = \hat{T} + \hat{V}$$

Here, \hat{T} is the kinetic energy operator and \hat{V} is the potential energy operator. The kinetic energy operator can be written in terms of the momentum operator if the classical formulae for kinetic energy and momentum are combined. The known momentum operator can then be substituted into the resulting expression.

$$T = \frac{1}{2}mv^2, \quad p = mv$$

$$\Rightarrow T = \frac{p^2}{2m}$$

$$\therefore \hat{T} = \frac{\hat{p}^2}{2m}$$

$$\hat{T} = \frac{(-i\hbar \frac{\partial}{\partial x})(-i\hbar \frac{\partial}{\partial x})}{2m} = \frac{i^2 \hbar^2}{2m} \left(\frac{\partial}{\partial x} \right) \left(\frac{\partial}{\partial x} \right) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

Note that $\frac{\partial^2}{\partial x^2}$ is the second partial derivative. We cannot derive a general expression for the potential energy operator in the same way because it depends on the system. Therefore, it is written as a function of the position, x .

$$\hat{V} = V(x)$$

These expressions for the potential and the kinetic energy operators can be added to find \hat{H} .

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

2.2.4 Eigenfunctions and Eigenvalues in Quantum Mechanics

The third postulate of quantum mechanics is that if a classical observable is measured, the only values that the observable can take are the eigenvalues of the corresponding operator. This postulate finally makes sense of the Schrödinger equation.

$$\hat{H}\psi = E\psi$$

The equation represents the Hamiltonian operator, \hat{H} , acting on the wavefunction, ψ , and giving back the same ψ multiplied by a constant, E . Therefore, to solve the Schrödinger equation, the eigenfunctions and eigenvalues of \hat{H} must be found. The eigenvalues, from the third postulate, give the measurable values of the classical observable corresponding to \hat{H} , and so are effectively the allowed total energies of the system, E . The eigenfunctions, ψ , are the wavefunctions corresponding to those values of energy.

2.2.5 The Wavefunction

There is no precise definition of the wavefunction, but there are certain useful interpretations, the most common being the Born interpretation. This states that the square of the wavefunction gives a probability density. For a wavefunction associated with a particle, this can be used to calculate the probability that a particle is found in a particular place. If, in a region of space, the probability density is $p(x)$, then the probability of finding the particle there is given by $p(x)dx$, where dx is the 'size' of that region. In three dimensions this would instead be $p(x, y, z)dV$.



Probability of finding particle between x and $x + dx = p(x)dx = |\psi(x)|^2 dx$

The total probability of finding the particle anywhere in space is 1, so the sum of the probabilities at every point in space must equal 1. This is represented mathematically as an integral.

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

A wavefunction that obeys this is said to be normalised, and any wavefunction can be normalised by multiplying it by some normalisation constant, N .

$$\int_{-\infty}^{\infty} N^2 |\psi(x)|^2 dx = 1$$

The Born interpretation imposes some restrictions on the wavefunction:

- The wavefunction must be single-valued because it does not make sense for a particle to have two different probabilities of being somewhere.

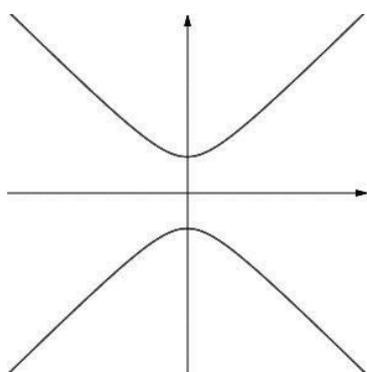


Figure 3 - A multi-valued function. This could not be a wavefunction.

- The wavefunction must be continuous because a break in the wavefunction would lead to a particle effectively having an undefined probability of being somewhere.

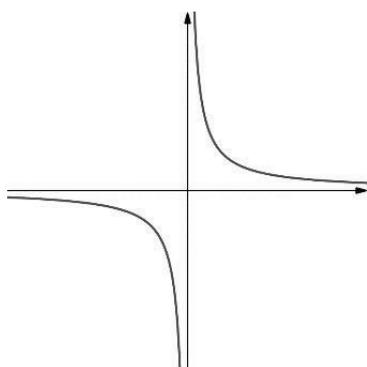


Figure 4 - A discontinuous function. This could not be a wavefunction.

- The wavefunction must be able to be normalised, so must have a finite integral over all space.

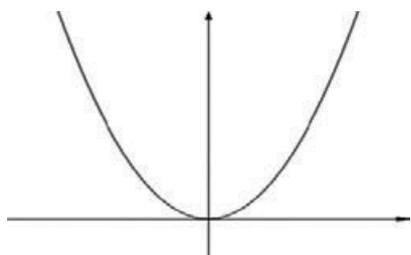


Figure 5 - A function with an infinite integral. This could not be a wavefunction.

2.2.6 Solving the Schrödinger Equation

The Schrödinger equation can be solved for several systems, including the harmonic oscillator and rigid rotor. The system we are going to solve it for is called ‘particle in a box’ which consists of a particle travelling in one dimension between $x = 0$ and $x = L$. In this region, the potential energy is zero and outside this region, the potential energy is infinite. This means that the particle cannot leave this region so perhaps a more suitable name would be ‘particle in an endless hell from which it can never escape’.

As the particle always experiences zero potential energy, the Hamiltonian operator is equal to the kinetic energy operator.

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

Using this, the Schrödinger equation for the system can be written.

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) = E\psi(x)$$

We are looking for a function whose second derivative is itself multiplied by a constant. Luckily, this has been solved many times before, so we can take a very well-informed guess at the solution.

$$\psi(x) = A \cos(kx) + B \sin(kx)$$

The constants A , B , and k are to be determined. We can now differentiate this function twice.

$$\frac{\partial}{\partial x} (A \cos(kx) + B \sin(kx)) = -kA \sin(kx) + kB \cos(kx)$$

$$\begin{aligned} \frac{\partial^2}{\partial x^2} (A \cos(kx) + B \sin(kx)) &= \frac{\partial}{\partial x} (-kA \sin(kx) + kB \cos(kx)) \\ &= -k^2 A \cos(kx) + k^2 B \sin(kx) \end{aligned}$$

$$\therefore \frac{\partial^2}{\partial x^2} \psi(x) = -k^2 \psi(x)$$

This can now be substituted into the Schrödinger equation.

$$-\frac{\hbar^2}{2m} (-k^2 \psi(x)) = E\psi(x) \Rightarrow \frac{\hbar^2 k^2}{2m} \psi(x) = E\psi(x) \Rightarrow E = \frac{\hbar^2 k^2}{2m}$$

We have derived an expression for the allowed energy levels, which depends on the constant, k . Applying boundary conditions, outside the interval $[0, L]$ there is no probability of finding the particle, so the wavefunction must be zero at $x=0$ and $x=L$.

$$\psi(0)=0 \Rightarrow A\cos(0)+B\sin(0)=0 \Rightarrow A=0$$

$$\psi(L)=0 \Rightarrow B\sin(kL)=0$$

The constant B cannot be zero or the wavefunction would be zero everywhere so $\sin(kL)$ must equal zero. For $\sin x$ to equal zero, x must be an integer multiple of π .

$$kL = n\pi \Rightarrow k = \frac{n\pi}{L}, \quad n = 0, \pm 1, \pm 2, \pm 3, \pm 4 \dots$$

This expression for k can be inserted into the expressions for the wavefunction and the allowed energy levels.

$$\psi_n(x) = B \sin\left(\frac{n\pi x}{L}\right)$$

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

If $n=0$, then the wavefunction is simply zero everywhere so this value is disallowed. If n is negative, the wavefunctions are the positive wavefunctions multiplied by -1 . The square of the wavefunction is, therefore, the same and so these values can also be ignored.

Our final solution to the Schrödinger equation can now be written.

$$\psi_n(x) = B \sin\left(\frac{n\pi x}{L}\right), \quad E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}, \quad n = 1, 2, 3 \dots$$

There is still an undetermined constant, B , which can be worked out by normalising the wavefunction. This process will not be covered here as the important result is the allowed energy levels, but the result is that

$$B = \sqrt{\frac{2}{L}}$$

SECTION 3 ATOMIC AND MOLECULAR ORBITALS

3.1 A HISTORY OF ATOMIC STRUCTURE

3.1.1 The Discovery of The Electron

In the late 19th century, there was great interest in cathode rays, which were created when a large potential difference was applied across a vacuum tube. In 1897, J. J. Thomson directed a stream of these rays between two charged plates and they deflected towards the positively charged plate. He concluded that the rays were made of negatively charged particles, electrons. From the magnitude of the deflection of the rays in electric and in magnetic fields, Thomson calculated the mass of the electron as only $\frac{1}{1836}$ the mass of a proton.

Thomson then suggested a model for the atom called the plum pudding model. This was based on the knowledge that atoms contained electrons but must also contain positive charge for the overall atom to be neutral. It consists of electrons distributed within a positively charged medium.

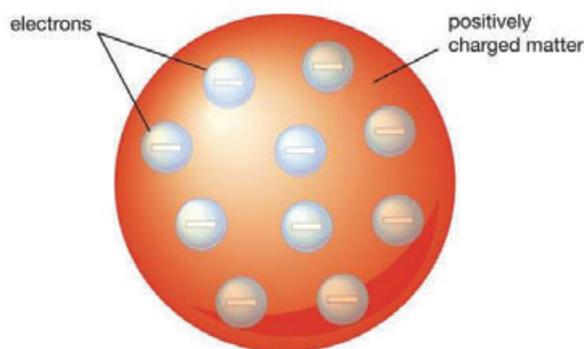


Figure 6 - The plum pudding model of the atom.

3.1.2 The Discovery of the Nucleus

In 1909, Ernest Rutherford and two fellow scientists Geiger and Marsden conducted an experiment in which a stream of alpha particles was fired at a very thin gold foil, and the angle of deflection of each alpha particle was measured. If the plum pudding model had been true, the alpha particles would have been deflected by a very small angle. However, while the majority passed through almost undeflected, a small fraction of the alpha particles was deflected by a large angle.

The conclusion was that Thomson's model was incorrect. In Rutherford's new model, most of the atom was empty space apart from a tiny sphere of positive charge in the centre of the atom, the nucleus, surrounded by orbiting electrons.

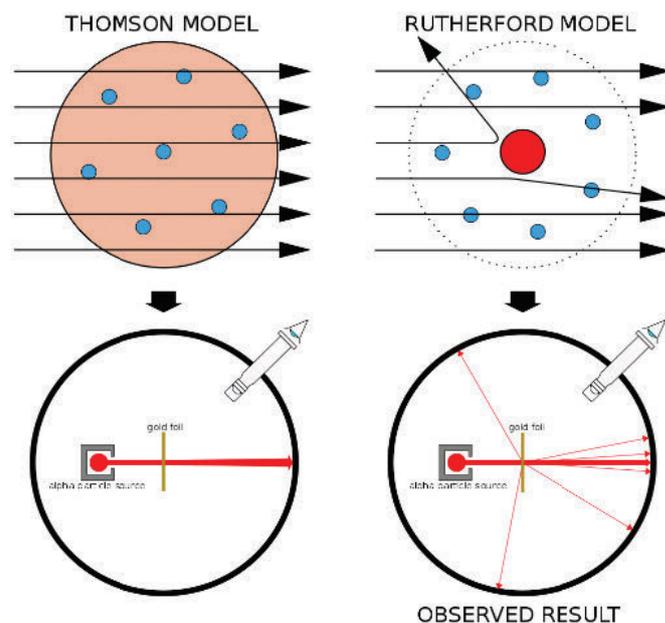


Figure 7 - A diagram of the Geiger-Marsden experiment.

3.1.3 The Bohr Model

The flaw with Rutherford's model was that the orbiting electrons, according to classical physics, would constantly emit electromagnetic radiation, and therefore lose energy and spiral into the nucleus in 10^{-16} picoseconds. This would make atoms inherently unstable.

In 1913, Niels Bohr proposed a new model to overcome this issue. He put forward three postulates:

1. Electrons revolve around the nucleus in stable orbits without radiating energy. These orbits are at certain discrete distances from the nucleus.
2. These discrete distances are such that the angular momentum, l , of an electron is an integer multiple of the reduced Planck's constant.

$$l = n\hbar, \quad n = 1, 2, 3 \dots$$

The smallest possible orbital radius, occurring when $n = 1$, is called the Bohr radius, a_0 .

3. An electron can only change its energy by jumping between orbits, either emitting or absorbing electromagnetic radiation of a frequency given by the Planck relation.

$$\Delta E = h\nu$$

This model of the atom quantises the energy levels of the electrons and can accurately predict the frequency of the lines in the emission spectrum of hydrogen. But just like the other models, it eventually was replaced by the modern theory of atomic orbitals.

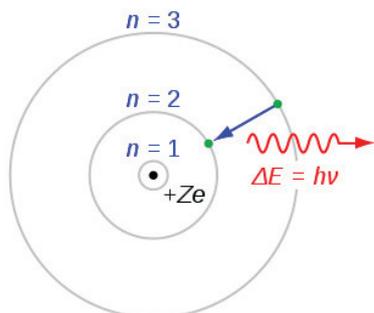


Figure 8 - Diagram showing an electron losing energy via emission of a photon.

3.2 ATOMIC ORBITALS

3.2.1 An Introduction to Orbitals

In Bohr's model, we know the electron's exact distance from the nucleus and its momentum. This violates Werner Heisenberg's uncertainty principle. We will not derive this, but it means we can never know both the position and momentum of any particle with complete accuracy. The product of their uncertainties must be greater than or equal to half of the reduced Planck's constant.

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

To solve this issue, the electrons must be described by wavefunctions. This means only knowing the probability of an electron being somewhere, not exactly where it is, no longer violating the uncertainty principle. These wavefunctions are atomic orbitals.

3.2.2 A Mathematical Description of Orbitals

The Schrödinger equation can be used to find mathematical expressions for the atomic orbitals. Unfortunately, it can only be solved exactly for single-electron systems as with multiple electrons there are too many interactions to deal with. However, these solutions do provide a good description of atomic orbitals in general.

For atomic orbitals, it is much easier to use polar coordinates than Cartesian coordinates. Cartesian coordinates use the variables x , y and z . Polar coordinates use the distance from the origin r , and two angles, θ and ϕ .

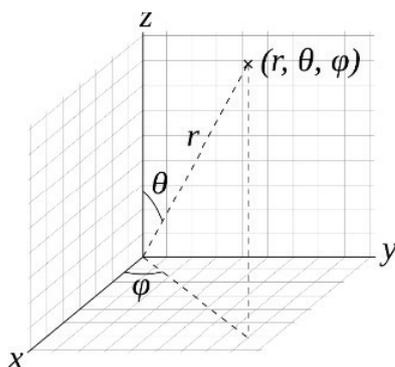


Figure 9 - Diagram showing polar coordinates.

When the Schrödinger equation is solved for a hydrogen atom, each wavefunction is characterised by three quantum numbers, similar to how the particle in a box wavefunction was characterised by n :

1. The principal quantum number, n , takes values 1, 2, 3...
2. The angular momentum quantum number, l , takes values 0, 1, 2..., $n-1$
3. The magnetic quantum number, m_l , takes values $-l, \dots, -1, 0, +1, \dots, +l$.

The principal quantum number determines the shell the electron is in and can completely determine the energy of a hydrogen orbital.

$$E_n = -\frac{Z^2 R_H}{n^2}$$

The nuclear charge, Z , is simply 1 for hydrogen and the Rydberg constant, R_H , has a value of 2.180×10^{-18} J. The energy is negative because a free electron is said to have zero energy and when bound by a nucleus it has less energy.

The principal and angular momentum quantum numbers determine the subshell an electron is in. For each value of l there is a corresponding letter, $l=0$ is s , $l=1$ is p , $l=2$ is d and $l=3$ is f . The possible values of l mean that in the first shell there is only an s subshell, in the second only s and p subshells and so on.

The principal, angular momentum and magnetic quantum numbers determine the orbital the electron is in. For the s subshells, m_l can only be 0 so there is one s orbital per subshell. For the p subshells, m_l can be $-1, 0, \text{ or } 1$, so there are three p orbitals per subshell. In the same way, there are five d and seven f orbitals per subshell. The orbitals are distinguished by a subscript. For example, $2p_x, 2p_y$ and $2p_z$ are the three p orbitals in the second shell.

The wavefunctions of hydrogen can be written as the product of a radial part, R , and an angular part, Y .

$$\psi_{n,l,m_l}(r, \theta, \phi) = R_{n,l}(r) \times Y_{l,m_l}(\theta, \phi)$$

The probability of an electron being found at a certain distance, r , from the nucleus can be calculated by multiplying the probability density of a point at that distance from the nucleus, $p(r)$, by the surface area of a sphere of that radius.

$$\text{Surface area of sphere} = 4\pi r^2$$

$$\text{Probability density of electron at radius } r = 4\pi r^2 p(r)$$

From the Bohr interpretation, the probability density, $p(r)$, is the square of the wavefunction. This defines the radial distribution function, $P(r)$, which is effectively a measure of the electron densities at different radii.

$$P(r) = 4\pi r^2 |\psi(r)|^2$$

3.2.3 A Closer Look at the s Orbitals

The simplest orbital is the $1s$ orbital, whose wavefunction we will consider now.

$$\psi_{1s} = N_{1s} e^{-r/a_0}$$

N_{1s} is a normalisation constant whose value is not important and a_0 is the Bohr radius. The value of the wavefunction only depends on the distance from the nucleus, so the orbital has spherical symmetry. The wavefunction has a maximum in the centre of the nucleus and decays exponentially outwards. The radial distribution function has a maximum at $r=a_0$, so the electron density is highest at this radius.

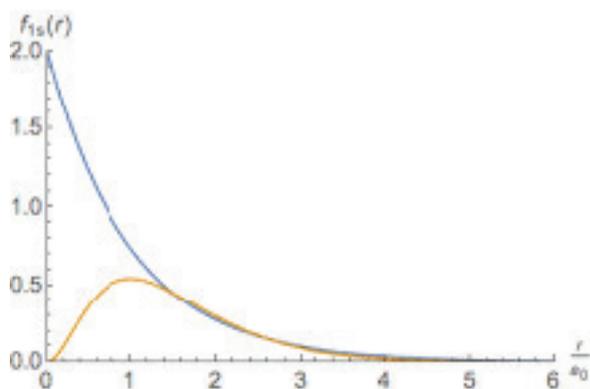


Figure 10 - Graph of the 1s wavefunction, blue, and radial distribution function, orange.

The issue with depicting orbitals on paper is that there are not enough dimensions. There are several ways of overcoming this, but each has its flaws. The one we are going to use is created by taking a cross-section through the orbital and plotting large numbers of dots based on the value of the wavefunction. The denser the dots, the higher the value of the wavefunction.

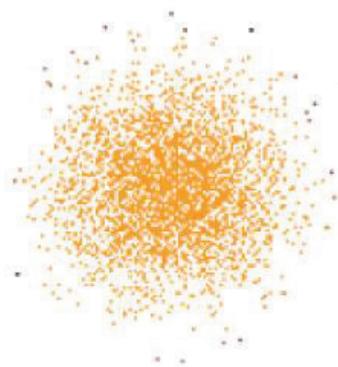


Figure 11 - Dot representation of the 1s orbital.

The wavefunction of the 2s orbital is slightly more complex than that of the 1s.

$$\psi_{2s} = N_{2s} \left(2 - \frac{r}{a_0} \right) e^{-\frac{r}{2a_0}}$$

Just like the 1s, this orbital is spherically symmetric. To compare the 2s orbital to the 1s their radial distribution functions can be plotted on the same graph.

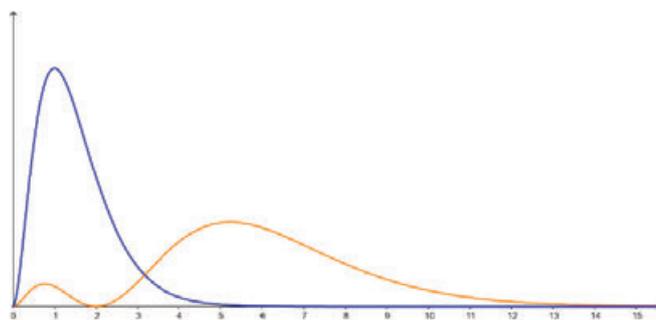


Figure 12 - Graphs of the radial distribution functions of the 1s, blue, and 2s, orange.

The main difference is that the 1s has higher electron density nearer the nucleus, and the 2s is more spread out and effectively larger. At $2a_0$ there is no electron density in the 2s orbital, which is called a node.

The dot representations can also be placed next to each other for comparison. Note that the blue colour represents a negative value of the wavefunction.

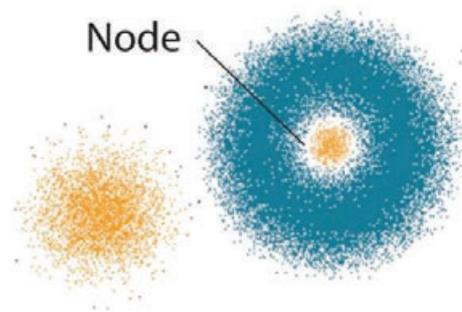


Figure 13 - Dot representations of the 1s and 2s.

The wavefunction of the 3s is again more complex than the previous wavefunctions.

$$\psi_{3s} = N_{3s} \left(27 - 18 \left(\frac{r}{a_0} \right) + 2 \left(\frac{r}{a_0} \right)^2 \right) e^{-\frac{r}{3a_0}}$$

We can plot the graph of the radial distribution function compared with the 1s and 2s and show the dot representation of the 3s.

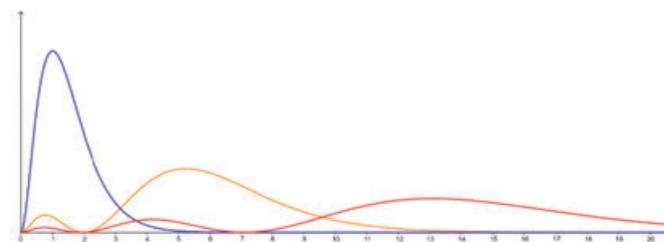


Figure 14 - Graph of the radial distribution functions of the 1s, 2s, and 3s.

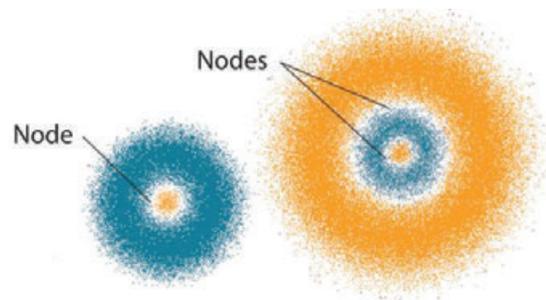


Figure 15 - Dot representations of the 2s and 3s.

From these, we can see that the 3s is larger still than the 2s orbital and that the 3s flips sign twice at two nodes. It should now be easy to predict the shape of the s orbitals for higher values of n .

3.2.4 A Closer Look at the p Orbitals

The p orbitals have more interesting shapes than the s orbitals as they no longer have spherical symmetry. We will look first at the radial part of the 2p orbitals.

$$R_{2p} = N_{2p} \left(\frac{r}{a_0} \right) e^{-\frac{r}{2a_0}}$$

To understand this, we can plot the radial distribution function of the 2p orbitals compared with the 1s and 2s.



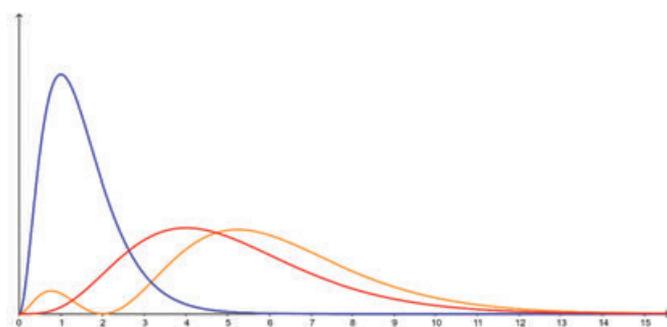


Figure 16 - Graph of the radial distribution functions of the 1s, blue, 2s, orange, and 2p, red.

It is a similar size to the 2s orbital, which should not be surprising as it has the same energy. It has no radial nodes, but it does have another type of node not seen in the radial part. The angular part depends on the particular p orbital.

$$Y_{p_z} = \cos(\theta), \quad Y_{p_x} = \sin(\theta) \cos(\phi), \quad Y_{p_y} = \sin(\theta) \sin(\phi)$$

Explaining what these mean mathematically can get confusing, so we will simply look at the result using the dot representation.

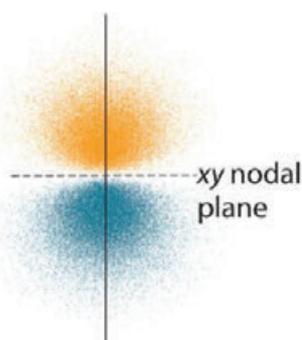


Figure 17 - Dot representation of the $2p_z$.

Each orbital has a nodal plane, shown in the diagram by a dotted line. Each side of this dotted line the wavefunction has the opposite sign. It turns out that each orbital has cylindrical symmetry, meaning it is symmetrical by rotation about a certain axis. The $2p_z$ lies along the z-axis and so on. Going into detail discussing any more orbitals is unnecessary for our future discussions so they will be left here.

3.2.5 Multi-Electron Atoms

For more complex atoms, we are adding electrons and increasing the nuclear charge. It is impossible to solve the Schrödinger equation analytically for these systems, so approximations and numerical methods are used to find the wavefunctions.

The way electrons occupy the orbitals is governed by their energy and the Pauli exclusion principle. An electron in hydrogen will usually occupy the lowest energy orbital, the 1s, but in multi-electron atoms, the electrons start to occupy different orbitals. This is because the Pauli exclusion principle prevents two electrons from having identical quantum numbers. There is a quantum number that we have not mentioned yet, spin. Electrons can either have a spin of $+\frac{1}{2}$ (spin-up) or $-\frac{1}{2}$ (spin-down). The result is that at most two electrons can occupy any orbital, as long as they have opposite spin. Therefore, electrons fill up the orbitals two at a time from lowest energy to highest energy.

The energies of the orbitals change in multi-electron atoms such that

those with the same n no longer need have the same energy. We will not go into a detailed discussion as to why this is, but we will show a graph of the energies of some of the orbitals as you increase the atomic number.

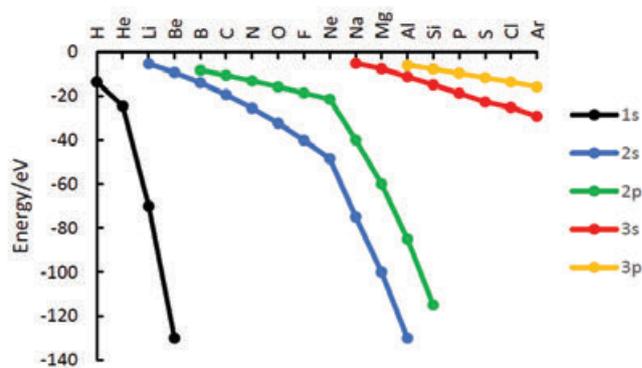


Figure 18 - Graph of the energies of orbitals in atoms of the first 18 elements.

The unit of electron volts, eV , makes the numbers easier to deal with as $1eV = 1.60 \times 10^{-19} J$. When the 1s orbital is full, the electrons then go into the 2s as this is actually lower in energy than the 2p. Then they go into the 2p, then the 3s, and so on. The results can be summarised in an electron configuration. For fluorine, it would be $1s^2 2s^2 2p^5$. This shows that there are two electrons in both the 1s and 2s subshells, and five in the 2p subshell.

3.3 DIATOMIC MOLECULAR ORBITALS

3.3.1 The Simple Case – H_2^+

Due to the presence of only one electron in H_2^+ , it is possible to solve the Schrödinger equation and the result is a molecular orbital (MO). MOs are filled up by electrons in order of increasing energy, just like atomic orbitals (AOs). For molecules with multiple electrons, some rules can be used to guess the form of the MOs and their relative energies, all of which can be derived from quantum mechanics.

One simple approach is called the linear combination of atomic orbitals, LCAO. This takes the algebraic sum of the AOs at every point in space to construct the MO.

$$MO = c_1(AO1) + c_2(AO2)$$

The constants, c_1 and c_2 , are orbital coefficients which can be determined through detailed quantum mechanical calculations. In the H_2^+ molecule, it would make sense for the lowest energy MO to be constructed from a combination of the two 1s orbitals. It turns out that there are two MOs formed from the combination of these AOs. For the first, $c_1 = c_2 = 1$ and for the second, $c_1 = 1, c_2 = -1$.

$$MO1 = N_1(1s \text{ of first atom} + 1s \text{ of second atom})$$

$$MO2 = N_2(1s \text{ of first atom} - 1s \text{ of second atom})$$

Again, N_1 and N_2 are normalisation constants. When the atoms are far apart, the MOs will effectively be identical in shape to the AOs. At shorter distances, MO1 will contain a region between the nuclei where the AOs are adding together and producing high electron density, called constructive overlap. For MO2, the AOs are subtracting and producing low electron density, called destructive overlap. Halfway between the nuclei, there will be a node of zero electron density.

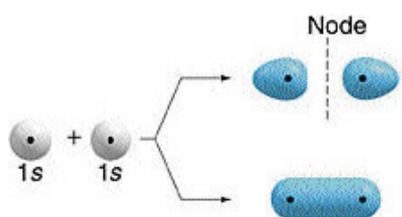


Figure 19 – H_2^+ molecular orbitals.

In H_2^+ , the lowest energy MO turns out to be MO1, so the electron occupies this orbital. This creates high electron density between the nuclei and pulls them towards each other until the attraction balances the repulsion of the nuclei. This is a chemical bond and so MO1 is described as a bonding orbital. If the electron were for some reason to be MO2, then the low electron density between the nuclei means that the repulsive force is strong, and the electron density either side of the nuclei pulls them apart. For this reason, MO2 is described as an antibonding orbital.

Molecular orbitals can be classified using symmetry. In H_2^+ , the orbitals are symmetric by rotation about the internuclear axis, and so are called σ orbitals. The only other type of orbital we will meet is one where rotation by 180° about the internuclear axis flips the sign of the wavefunction. This is called a π orbital. Bonds formed by these orbitals are called σ and π bonds, respectively. Antibonding orbitals are given an asterisk, for example σ^* .

The energies of MOs can be represented on a MO diagram. The horizontal lines represent orbitals, with those at the sides being the original AOs, and those in the centre being the MOs. At large separation, the lines are the same level as the MOs are equivalent to the AOs. As the atoms get closer, the bonding MO lowers in energy and the antibonding MO increases in energy.

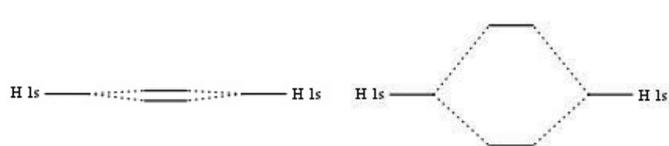


Figure 20 - MO diagrams for overlap of $1s$ orbitals at large (left) and small (right) separation.

3.3.2 More Complex Cases – H_2 , He_2^+ , and He_2

The MOs can be filled in a similar way to how AOs are filled. Two electrons are placed in each orbital with opposite spin, starting with the lowest energy orbital. For the simple case of two $1s$ orbitals forming a σ and a σ^* orbital, it can be seen that the first two electrons fill the σ and the next goes into the σ^* . This can be represented using MO diagrams.

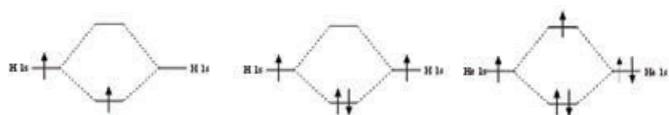


Figure 21 - Molecular orbital diagrams of H_2^+ (left), H_2 (centre) and He_2^+ (right).

If we were to add another electron it would go into the σ^* orbital. It turns out that the σ^* orbital is slightly more raised in energy than the σ is lowered. This would mean that going from two He atoms to an He_2 molecule would lead to a net increase in energy, showing why helium does not form diatomic molecules.

3.3.3 Rules of Forming Molecular Orbitals

We will not cover how these rules are derived but they are very useful for constructing MOs from AOs.

1. If n AOs are combined, n MOs are formed.
2. AOs can only combine if they have the correct symmetry.
3. AOs that are closer in energy have a larger interaction when forming MOs.
4. AOs which are closer in energy to an MO contribute more to it.
5. AOs can only interact strongly if their sizes are compatible.

The first of these is quite simple to understand. If we pull apart a molecule, the MOs will steadily become AOs. Since this must be a continuous process, the number of orbitals cannot change.

To understand the second, we will cover a disallowed interaction. If we try to combine a $2s$ and a $2p_x$ orbital, taking the internuclear axis to be the z -axis, then one lobe of the $2p_x$ orbital will constructively overlap with the $2s$ and the other will destructively overlap with it. The overlaps will be equal and opposite and so the total overlap will be zero, so these AOs do not form an MO. For a $2s$ and $2p_z$, this is not a problem and so an MO can be formed.



Figure 22 - Diagram showing the disallowed overlap between $2s$ and $2p_x$ (left) and allowed overlap between $2s$ and $2p_z$ (right).

The third rule can be easily explained with MO diagrams.



Figure 23 - MO diagrams showing how AOs of the same energy (left) combine compared to AOs of different energies (right).

It can be seen that as the difference in energy between the AOs increases, the MOs become closer in energy to the original AOs, so the interaction decreases. The fourth rule is self-explanatory and simply means that the higher energy AO contributes more to the antibonding MO and vice versa.

The fifth rule is also a result of the overlap as, if the two orbitals differ greatly in size, then the overlap will not be effective, and the AOs will not interact strongly.

3.3.4 Combining Different Atomic Orbitals

When $2s$ orbitals are combined the result is simple and we end up with another σ and σ^* of higher energy than with a combination of $1s$ orbitals. When $2p_z$ orbitals are combined, as these lie on the internuclear axis, we get another σ and σ^* , which are higher in energy still. They are, however, slightly different from the σ MOs created from s orbitals.

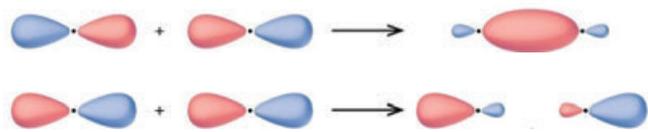


Figure 24 - Diagram showing the bonding (top) and antibonding (bottom) MOs created from two $2p_z$ orbitals.

When $2p_x$ and $2p_y$ orbitals are combined, the resulting MOs are π and π^* . These do not have cylindrical symmetry and so look more complex than the σ orbitals.

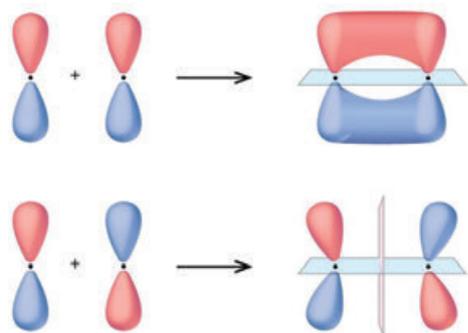


Figure 25 - Diagram showing the bonding (top) and antibonding (bottom) MOs created from two $2p_x$ or $2p_y$ orbitals.

With this knowledge, we can draw an MO diagram displaying the bonding between many different atoms. As an example, we will draw one for the nitrogen molecule. For simplicity, we will assume that only interactions between identical orbitals can occur, although in reality the s and p orbitals can interact.

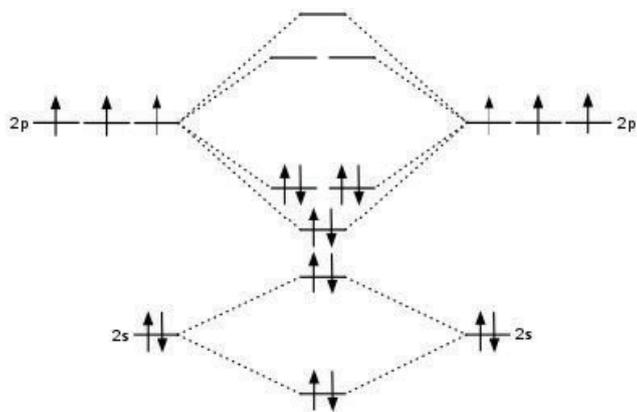


Figure 26 - MO diagram for the N_2 molecule.

The $1s$ interactions have been ignored as they are much lower in energy. The most important interactions are those of the p orbitals, and the order of energy of their MOs is σ , π , π^* , σ^* . The electrons shown fill four bonding MOs and one antibonding, giving N_2 an overall triple bond.

SECTION 4 BONDING IN ORGANIC MOLECULES AND COLOUR

4.1 HYBRIDISATION

4.1.1 An Introduction to Hybrid Orbitals

When describing bonding in organic molecules, using the molecular orbitals described in the last section would be almost impossible.

For more than a few atoms there are too many interactions to deal with, and the molecular orbitals become very difficult to interpret. Hybridisation is a different approach that helps solve this issue.

Hybridisation is the mixing of AOs to creating hybrid atomic orbitals (HAOs). These HAOs often combine to form much more simple MOs. For example, with methane, the issue with using the full MO approach is that the AOs do not point directly towards the four hydrogen atoms. The $2s$ points equally in all directions and the $2p$ orbitals point at right angles, not at the tetrahedral angle of 109.5° . The hybrid approach allows for four simple HAOs that point directly to each hydrogen, creating simple MOs.

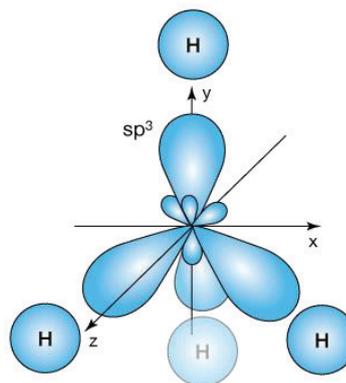


Figure 27 - Diagram showing the HAOs of methane.

4.1.2 Different HAOs – sp^3 , sp^2 , and sp

In organic molecules, we are usually considering bonding to carbon atoms. If the carbon atom is bonded to four other atoms, four different HAOs need to be formed just like in methane. The way this is done is by directly combining the single $2s$ orbital with the three $2p$ orbitals. The new orbitals are sp^3 hybridised. Each of these are identical and are separated by 109.5° .

The energy of this hybrid orbital is between the energy of the $2s$ and $2p$ orbitals and turns out to be similar in energy to the $1s$ orbital of a hydrogen atom. We can draw an MO diagram for the combination of an sp^3 HAO with a hydrogen $1s$ AO. There is one electron contributed from each orbital and so both go into the bonding MO, forming a C-H bond.

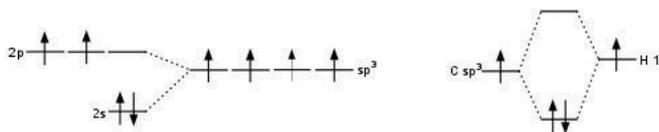


Figure 28 - MO diagrams showing the creation of sp^3 HAOs (left) and the creation of a C-H bond (right).

When a carbon is double bonded to an atom, we must use a different hybridisation. The required HAOs should be at 120° to each other and in the same plane. This can be done by combining the $2s$ orbital with only two of the $2p$ orbitals. This creates three sp^2 hybridised orbitals and a leftover $2p$ orbital. In the case of ethene, C_2H_4 , each carbon has two σ bonds to hydrogens created by a combination of the hydrogen $1s$ and an sp^2 HAO from the carbon. There is also a σ bond between the two carbons created by the head-on overlap of two sp^2 HAOs. Finally, the double bond is a π bond formed by the overlap of the leftover $2p$ orbitals.

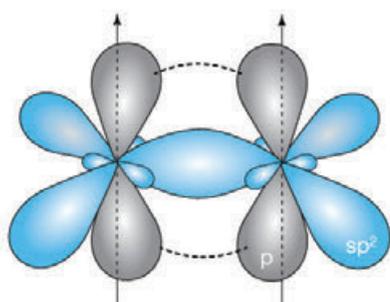


Figure 29 - Diagram showing the σ and π interactions in ethene.

Finally, when a carbon has a triple bond, it must be sp hybridised. This leaves two $2p$ orbitals that can generate two π bonds in addition to the σ bond, creating a triple bond. This can be used to describe the bonding in ethyne, C_2H_2 .

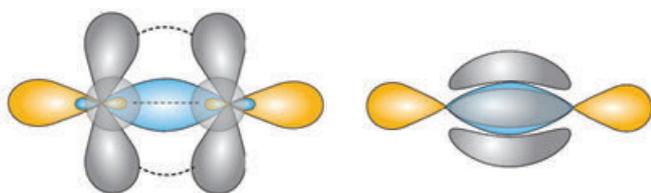


Figure 30 - Diagrams to show the interactions in ethyne. One helps show the σ bond (left) and one the π bonds (right).

4.2 DELOCALISATION AND CONJUGATION

4.2.1 Delocalised Bonding

So far, we have covered localised bonding, meaning that the bonding occurs between two atoms. This gives an accurate picture in most circumstances, but there are notable exceptions where this fails to explain certain properties of a molecule, giving rise to delocalised bonding.

One well-known example is benzene, a molecule with the molecular formula C_6H_6 . In 1865, August Kekulé proposed a structure for benzene.

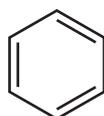


Figure 31 - Kekulé structure of benzene.

A double bond is stronger and therefore shorter than a single bond, so we would expect benzene to have alternating long and short bonds. However, it turns out that each bond length is identical and approximately halfway between that of a single bond and a double bond. This suggests that each bond is effectively one and a half bonds. This is because the electrons in the p orbitals of benzene are delocalised over all six carbon atoms equally, and so instead of alternating double and single bonds, a circle is drawn.



Figure 32 - Delocalised structure of benzene.

To represent delocalisation, multiple structures can be drawn with a double-headed arrow between them. This means that the molecule is somewhere between these two forms. The curly arrows here do not represent a reaction but simply that the electrons are delocalised around the ring.

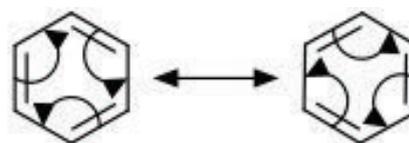


Figure 33 - Diagram showing the delocalisation in benzene.

As benzene chooses to adopt this delocalised form, we can conclude that delocalisation is a stabilising effect.

4.2.2 Delocalisation in Carbon Chains

Delocalisation is not confined to rings but shows up in many different organic molecules. For example, trans-hexatriene.

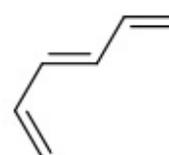


Figure 34 - Trans-hexatriene.

There are two main issues with a localised bonding description of this molecule. One is that the molecule should rotate freely about the single bonds, but it turns out to be planar. The other is that the single bonds are shorter than they should be and the double bonds slightly longer.

If we carry over the idea from benzene that the p orbitals can delocalise over the whole molecule, then we can understand why it is planar. If the molecule were not planar, the p orbitals would not overlap effectively. It adopts a planar form to maximise delocalisation and its stabilising effect.

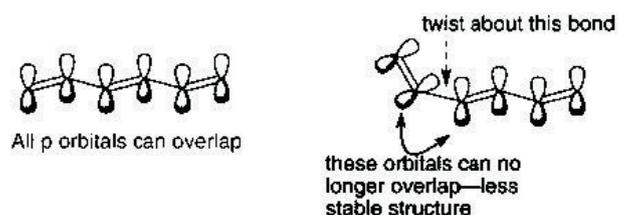


Figure 35 - Diagram showing why trans-hexatriene is planar.

Conjugation is the presence of alternating double and single bonds and it allows for p orbital delocalisation. Note that if two single bonds separate the double bonds, the p orbitals are too far away to overlap and if there are two double bonds directly next to each other, the p orbitals lie perpendicular to each other and cannot overlap. A clear example of an extended conjugated system is in β -carotene, the molecule that gives carrots their orange colour.

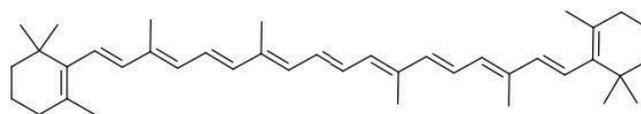


Figure 36 - The clear conjugated system in β -carotene.

4.2.3 Other Examples of Delocalisation

Delocalisation does not just occur over carbon atoms. A good example is in propenal.

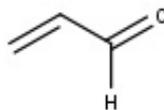


Figure 37 - Propenal.

There are two double bonds separated by a single bond, so this molecule is conjugated. The presence of an oxygen changes the energies of the p orbitals, but they still overlap. The resultant MO covering the whole molecule is not symmetric, but there is still delocalisation.

Charge on a molecule can create delocalisation where otherwise it would not be seen. An example is the allyl anion.

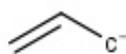


Figure 38 - Allyl anion.

There is only one double bond, but the rightmost carbon is sp^2 hybridised with a leftover p orbital, in which there are two electrons. This p orbital can delocalise with the p orbitals of the double bond. This delocalisation makes the anion symmetric.



Figure 39 - Diagram showing how delocalisation makes the allyl anion symmetric.

4.2.4 The Molecular Orbitals of Conjugated Systems

Now we can discuss the form of the MOs that the overlapping p orbitals create. To do this we will consider how the π and π^* MOs combine. One of the simplest examples is 1,3-butadiene.



Figure 40 - 1,3-butadiene.

We are combining two π and two π^* localised MOs, so we will create a total of four new delocalised MOs. The lowest energy combination will be when the two π MOs combine in phase (constructively), so there are no nodes. The next highest will be when the two π MOs combine out of phase (destructively), creating a node through the central bond. Then we combine the two π^* MOs in phase, creating two nodes. The highest energy orbital will be when the two π^* MOs combine out of phase.

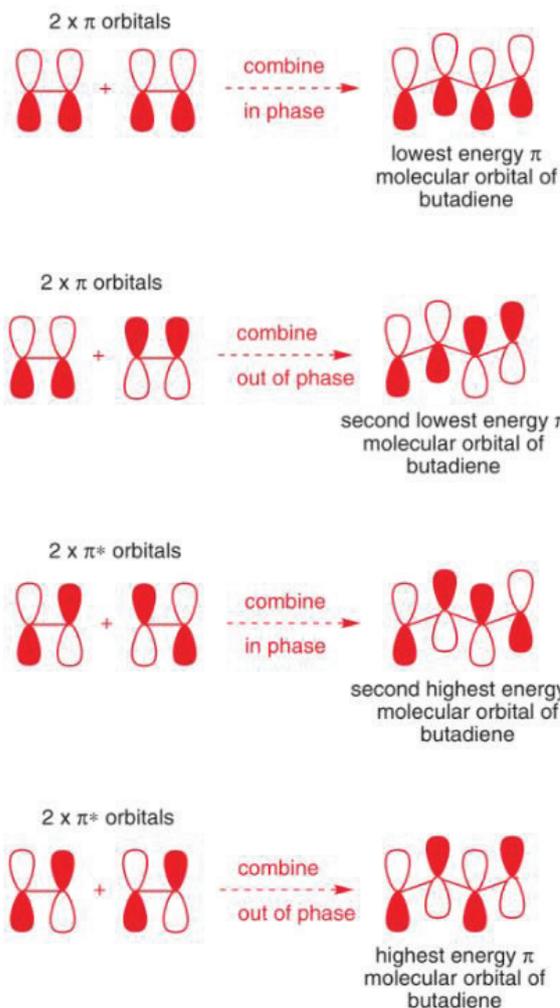


Figure 41 - Diagrams depicting how the π and π^* MOs combine.

This can be represented on an MO diagram. Notation is to label the new MOs ψ_1 , ψ_2 , ψ_3 , and ψ_4 in order of increasing energy.

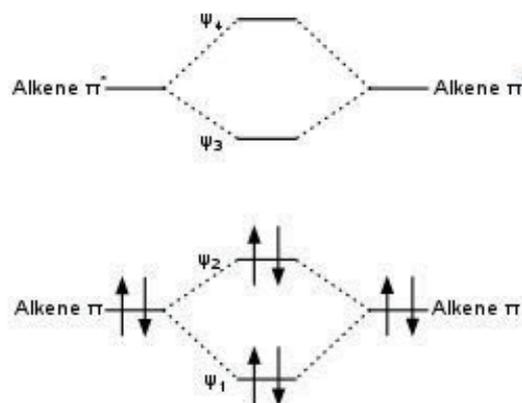


Figure 42 - MO diagram showing the energies of the MOs in butadiene.

The diagram has been filled with four electrons, two from each π orbital, and the total effect is a slight lowering of energy. The highest energy orbital with electrons in it is called the HOMO (highest energy occupied molecular orbital), and the lowest energy orbital without electrons in it is called the LUMO (lowest energy unoccupied molecular orbital).

4.3 COLOUR OF CONJUGATED SYSTEMS

4.3.1 Modelling Conjugated Systems with Particle in a Box

We can now explain the absorbance of visible light by conjugated systems. When light is shone on a molecule with a conjugated system, an electron can absorb a photon of the right frequency to jump from the HOMO of that conjugated system to the LUMO. The frequency of the light depends on the energy difference between the HOMO and LUMO via the Planck relation $\Delta E = h\nu$.

The energies of the HOMO and LUMO can be estimated using particle in a box. An electron moving through a conjugated system can be thought of as a particle moving from one end of the conjugated system to the other as the electron is effectively trapped within the molecule. For simplicity, we will deal only with conjugated systems in simple carbon chains.

4.3.2 Calculating the Colour of Molecules

We have already derived the energy levels for particle in a box.

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

We can turn this into a formula depending on the number of double bonds in a straight-chain conjugated system, k . The length of the system, L , can be approximated by taking the average bond length, R , which is approximately the mean of the C=C and C-C average bond lengths, and multiplying it by the total number of bonds in the chain, which is $2k - 1$.

$$L \approx (2k - 1)R$$

To work out the difference in energy between the HOMO and the LUMO, we must write n , the energy level, in terms of k . Each double bond contributes two electrons to the conjugated system, but there are two electrons per energy level and so for the HOMO, $n = k$. The energy level of the LUMO is therefore $n = k + 1$.

$$\begin{aligned} \Delta E &= E_{LUMO} - E_{HOMO} \\ &= \frac{\hbar^2 (k+1)^2 \pi^2}{2mL^2} - \frac{\hbar^2 k^2 \pi^2}{2mL^2} = \frac{\hbar^2 \pi^2}{2mL^2} ((k+1)^2 - k^2) = \frac{\hbar^2 \pi^2}{2mL^2} (2k+1) \end{aligned}$$

Into this, we can substitute the Planck relation, $\Delta E = h\nu = \frac{hc}{\lambda}$.

$$\Delta E = \frac{hc}{\lambda} = \frac{\hbar^2 \pi^2}{2mL^2} (2k+1) \Rightarrow \lambda = \frac{2mL^2 hc}{\hbar^2 \pi^2} (2k+1) = \frac{8mc}{h} \left(\frac{L^2}{2k+1} \right)$$

In this equation, m , the mass of an electron, h , c , and R are all constants. Given the number of double bonds, we have an equation that gives us the absorbed wavelength of light. The colour that the molecule appears will be the complementary colour to the absorbed colour.

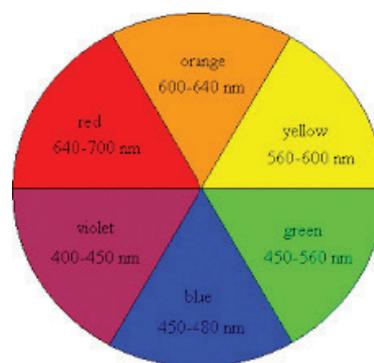


Figure 43 - A colour wheel can be used to easily work the colour of a molecule given the wavelength it absorbs.

Let us calculate values for the absorbed wavelength for $k = 1 - 5$.

No. Double Bonds	Absorbed Wavelength/nm
1	23
2	123
3	244
4	372
5	503

Figure 44 - Table showing the calculated absorbed wavelengths for 1-5 double bonds.

Past this, the calculated wavelength diverges from the actual value as this method is just an approximation. However, we are shown the very important point that a molecule must have a conjugated system of a reasonable length, at least five or six double bonds, to absorb in the visible spectrum. These extended conjugated systems turn out to be what give dyes their colour.

SECTION 5 TERMINOLOGY AND HISTORY OF DYES

5.1 SOME SIMPLE TERMINOLOGY

To avoid confusion in our later discussions of dyes, there are a few terms that should be defined.

- Dye – A water-soluble organic substance that is coloured and can impart colour to an object, e.g., betanin (found in beetroot).
- Pigment – A water-insoluble, coloured, inorganic substance, e.g., hematite (Fe_2O_3).
- Fastness – The resistance of a dye to being removed from a material by washing or by exposure to light or heat.

5.2 HISTORY OF DYES

5.2.1 Ancient History

Dyes have a very long history. The first appearance of dyes is debated but prehistoric rock paintings, done using pigments, dating back to thousands of years BC are believed to depict coloured garments. One of the oldest dyes is indigo, used in denim. The oldest example

of an indigo-dyed fabric is from 6000 years ago. The earliest written reference to dyeing is from China in 2600 BC.

In ancient civilisations, dyes were often seen as a luxury. Tyrian Purple was worth more than its weight in gold. It was extracted from sea snails and it is estimated that for 1g of the dye, about 8,500 snails must be used. Alexander the Great is said to have found old purple robes when he conquered Susa, Persia's capital, which are suspected to have had a value equivalent to \$6 million.



Figure 45 - Depiction of Justinian I wearing Tyrian Purple robes.

5.2.2 Pre-Synthetic Dyes

Before the 19th century, dyes were found purely from natural sources. In the 15th century, insects were often used as a source. For example, the dye carmine comes from the insect cochineal. In the 1600s, dyeing 'in the wood' was introduced which involved extracting dyes from wood chippings. Logwood and fustic dyes are examples.

Prior to the 18th century, bleaching was done using alkaline or acid baths, but this often took months. In 1774, Carl Scheele discovered a yellow-green gas that removed colour from certain objects, chlorine. Claude Berthollet was the first to suggest its use in bleaching fabrics. He also discovered sodium hypochlorite, the first commercial bleach. Since then, many bleaching chemicals have been discovered such as hydrogen peroxide.

5.2.3 Synthetic Dyes

The turning point in dye history was the year 1856. William Perkin, 18 at the time, was attempting to synthesise quinine. Organic synthesis, however, was poorly understood at this point. One of his attempts involved oxidising aniline using potassium dichromate. The structures of aniline and quinine are shown below, and it is clear that this was not going to work.

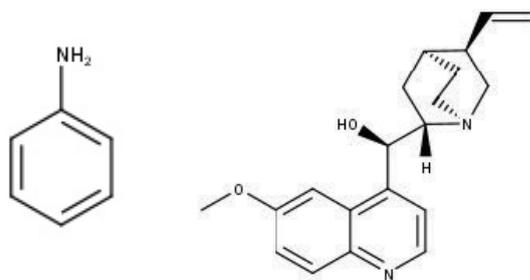


Figure 46 - Aniline (left) and quinine (right).

After this failed attempt, Perkin noticed a purple colour in his apparatus. Toluidine impurities in the aniline sample had reacted with the aniline, producing a variety of derivatives of mauveine differing only in the placement of methyl groups. These all absorbed light in the region 540-550nm due to the extended conjugated system, giving them their purple colour. A colour-coded structure of mauveine A is shown below, along with *o*-toluidine and *p*-toluidine. The green atoms are from *o*-toluidine, the red from aniline, and the blue from *p*-toluidine. The black bonds are those formed in the reaction.

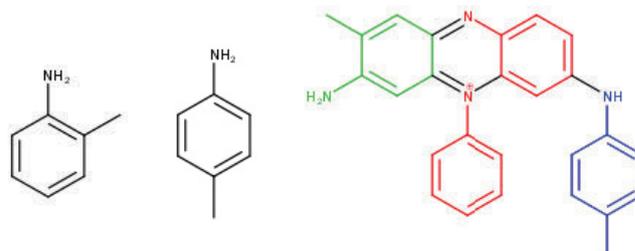


Figure 47 - The structures of *p*-toluidine (left), *o*-toluidine (centre) and mauveine A (right).

Perkin began mass-producing mauveine under the name aniline purple. From that point, discoveries in dye chemistry were being made frequently. In 1858, Peter Griess discovered the processes called diazotisation and coupling, reactions important in the synthesis of azo dyes. Ten years later, Graebe and Liebermann produced alizarin, the first natural dye to be produced synthetically. The first azo dye was successfully synthesised in 1880 by two English scientists, Thomas and Holliday. These are just a few of many discoveries made in the 19th and 20th centuries concerning the chemistry of dyes.

SECTION 6 STRUCTURE OF DYES

6.1 CHROMOPHORES AND AUXOCHROMES

6.1.1 Basic Structure

Graebe and Liebermann, in 1868, put forward the idea of dyes containing conjugated systems. In 1876 another German, Otto Witt, suggested a general structure of dyes consisting of a conjugated system of benzene rings with certain groups attached such as $-\text{NO}_2$, $-\text{C}=\text{O}$, or $-\text{N}=\text{N}-$, called the chromophore, and a polar group such as $-\text{OH}$ or $-\text{NH}_2$, called the auxochrome. The chromophore imparts colour to the dye and the auxochrome deepens that colour (shifts the absorption to a longer wavelength). A couple of examples are shown below with the chromophores coloured blue and the auxochromes red.

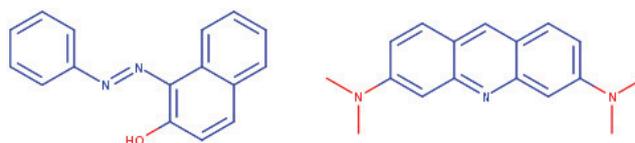


Figure 48 - The structures of Sudan I (left) and Acridine Orange (right).

6.1.2 Chromophores

Dyes are often built around a central chromophore, so certain groups in the chromophore can be used to classify the dye. Witt's idea of the chromophore, while generally correct, took a slightly restricted view of the possible structures it can take.

Azo dyes contain an -N=N- group in their chromophore. The groups attached to these nitrogens are often aryl groups. With the right substituents, they can absorb a wide range of wavelengths, but are mostly used for red, orange, and yellow dyes. Many azo dyes contain an $\text{-SO}_3\text{H}$ group as an auxochrome. This is mostly present as -SO_3^- in neutral conditions so azo dyes are often produced as salts, with the organic body of the dye being the anion.

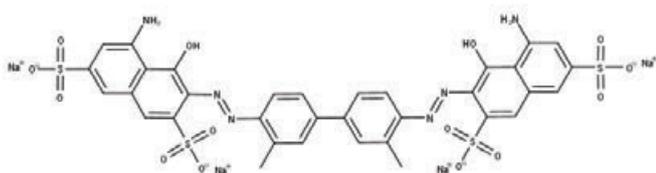


Figure 49 - The structure of Trypan Blue, an azo dye.

Arylmethane dyes are divided into two main subgroups, diarylmethane dyes and triarylmethane dyes. The backbones of these two groups are shown below.

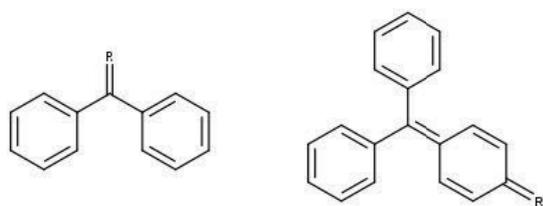


Figure 50 - Diarylmethane (left) and triarylmethane (right) general structure.

Auramine O is currently the only commonly used diarylmethane dye. Methyl violet dyes are triarylmethane dyes with $\text{-N(CH}_3)_2$ groups at the para position of at least two of the aryl groups. Fuchsine dyes can have primary or secondary amines at these positions. A final example is phenol dyes, where at least two aryl groups have -OH groups at their para positions. These phenol dyes often change colour with pH, for example, phenolphthalein. Many of these dyes, due to their amine groups, are basic and are often produced as salts with the organic body as the cation.

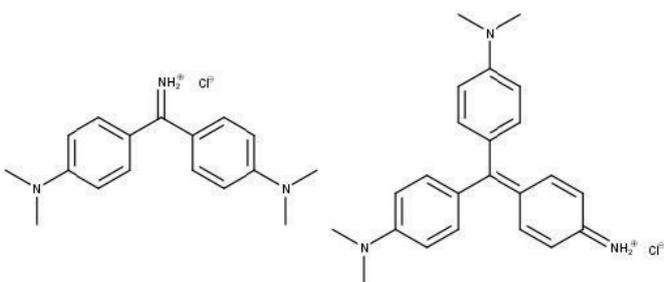


Figure 51 - The structures of Auramine O (left) and Methyl Violet 6B (right).

Anthraquinone dyes are built around an anthraquinone chromophore.

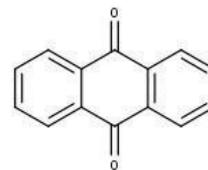


Figure 52 - Anthraquinone.

Anthraquinone is colourless and so auxochromes such as -OH are needed. Alizarin contains two -OH groups on the same aryl group. This structure allows alizarin to act as a pH indicator.

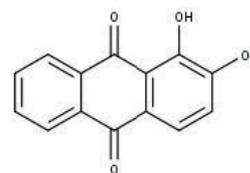


Figure 53 - The structure of alizarin.

Xanthenes-based dyes contain heterocycles, which in organic chemistry are rings containing elements other than carbon. Xanthene itself is not particularly useful, but when it is slightly altered it becomes a good chromophore.

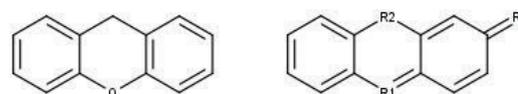


Figure 54 - The structures of xanthene (left) and a general xanthene derivative (right).

The main classes of xanthene-based dyes involve substitutions of R_1 and R_2 .

R1	R2	Dye Class
CH=	-S-	Thiopyronine
-CH=	-O-	Pyronine
-CH=	-NH-, -NMe-	Acridine
-N=	-S-	Thiazine
-N=	-O-	Oxazine
-N=	-NH-, -NMe-	Azine

Figure 55 - Table showing the dye classes in relation to the R groups.

These derivatives all have different uses. Oxazines and thiazines fade quickly in light on silks but are useful for dyeing acrylics. Mauve, the first synthetic dye, was an azine. Fluorescein is a type of fluorescent xanthene-based dye.

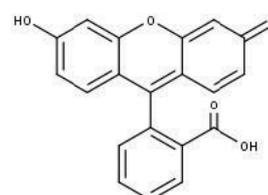


Figure 56 - The structure of fluorescein.

The phthalocyanines were first developed in the 20th century, more recently than the other classes. They are the synthetic analogues of chlorophyll and haemoglobin. Phthalocyanine itself is similar in structure to the common organic molecule, porphyrin.

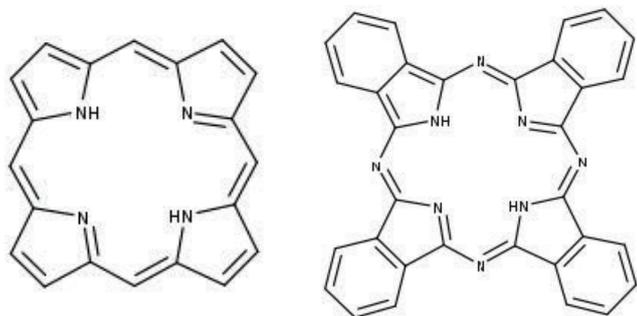


Figure 57 - The structures of porphyrin (left) and phthalocyanine (right).

Some of the carbons of phthalocyanine can be substituted for nitrogen, and some of the outer hydrogens for auxochromes such as $-OH$ or $-NH_2$ groups. This allows the colour of the dye to be finetuned. Phthalocyanines are often produced as metal complexes, with the most common metal ion being copper. For example, the dye Monostral Fast Blue G is simply phthalocyanine as its copper complex.



Figure 58 - The structure of Monostral Fast Blue G.

6.1.3 Auxochromes

Auxochromes usually contain a polar group with a lone pair. For example, $-OH$, $-NH_2$ and $-SH$. These donate electrons into the conjugated system and lengthen it, decreasing the energy difference between the HOMO and the LUMO, causing an absorbance shift to a longer wavelength known as a bathochromic shift.

There are certain examples which can cause a shift to a shorter wavelength, a hypsochromic shift. This is often due to the presence of carbonyl groups next to heteroatoms. However, we will not cover the details of how this works here.

Auxochromes can be divided into two groups, acidic and basic. This division mainly affects how a dye is applied. Nitrogen-based auxochromes are generally basic, and oxygen and sulphur-based auxochromes are generally acidic.

SECTION 7 APPLICATION AND BLEACHING

7.1 APPLICATION OF DYES

7.1.1 Material Structure

To understand how dyes are applied we must cover the chemical structure of certain materials.

Many fabrics, such as cotton, are made of plant fibres which are composed mainly of cellulose. Cellulose is a polymer of glucose and the repeat unit of cellulose is shown below. The chains are stacked on top of each other and attract each other via hydrogen bonds.

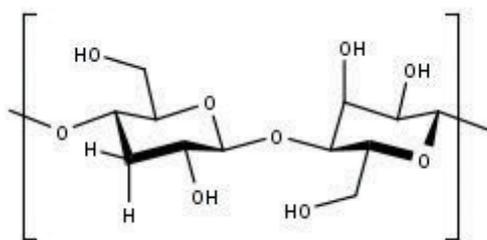


Figure 59 - The repeat unit of cellulose.

In all plant-based fibres, there are substances other than cellulose present such as lignin and pectin. This is not important, however, as the cellulose is abundant enough for a deep colour to be achieved anyway. For example, cotton is usually 94% cellulose and most plant fibres contain at least 60%. Rayon is a type of synthetic cellulose, and acetate rayon replaces some of the $-OH$ groups with $-OAc$ groups. Both of these are commonly used in the clothing industry.

Silk, and other animal fibres such as hair, wool and leather, are mainly composed of proteins. These are chains of amino acids joined by peptide bonds. For example, the main protein in silk is fibroin, generally consisting of the recurring sequence of amino acids Gly-Ser-Gly-Ala-Gly-Ala.

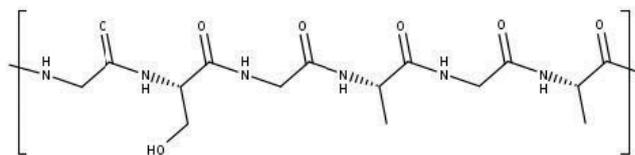


Figure 60 - Recurring sequence of amino acids in the protein fibroin.

In hair and wool, the main protein is keratin and in leather, it is collagen. Different proteins have different amino acid sequences. The amino acids often contain acidic, basic, and polar groups which serve as useful points for interacting with dyes molecules.

Synthetic fibres are usually polymers of some sort. Nylon, for example, is similar in structure to proteins, with amide groups separated by carbon chains of certain lengths. The polar amide groups serve as sites for interaction with dyes. Acrylics in their purest form are chains of hydrocarbons bearing nitrile groups. To improve dyeability, they are often polymerised in the presence of other molecules which add groups such as $-OH$. The structures of nylon-6 and a general acrylic polymer are shown below.

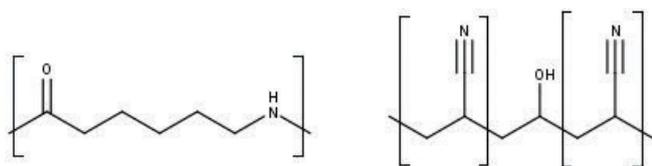


Figure 61 - The repeat unit of nylon-6 (left) and an acrylic polymer (right).

Some synthetic materials are difficult to dye. PET accounts for 50% of worldwide synthetic fibre production, and while it does contain polar groups that would serve as reasonable dyeing sites, the polymer chains are packed too close together for effective dyeing.

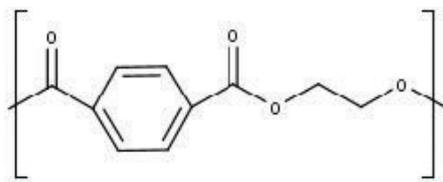


Figure 62 - The repeat unit of PET.

Tight chain packing leads to poor dyeability because dyeable fibres must be porous so that dye molecules can enter the fibre through pores and fix themselves to the chains. If these pores are too small, like in PET, then very few dye molecules can enter the material and the material is not easily dyed.

7.1.2 Dyeing Methods

There are multiple ways in which dyes can bond to fibres. These depend on both the material and the type of dye being used.

Direct dyes are applied simply by placing the material in a hot, aqueous solution of the dye. The temperature improves dye solubility, and direct dyes must be water-soluble. For this reason, they usually contain ionic or polar groups. Direct dyes can be applied to most fabrics, except tightly packed ones such as PET. The main bonding interactions are between ionic or polar groups of the fibre and the dye. Direct dyes are often large, resulting in strong intermolecular forces of attraction (dispersion forces) between the dye and the fibre, further strengthening its attachment.

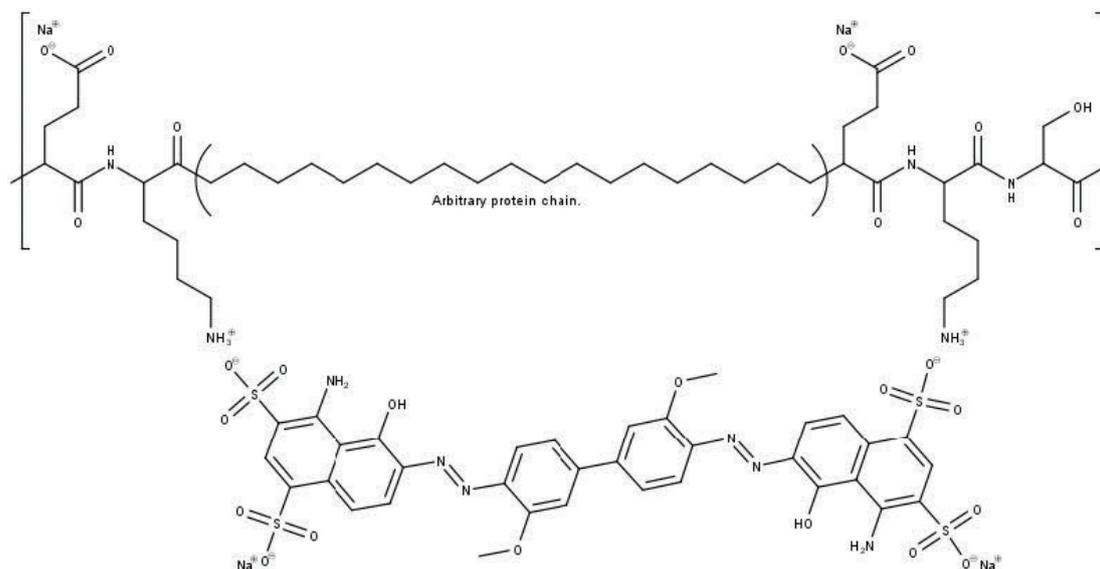


Figure 63 - Example of an ionic interaction between an arbitrary protein and the dye Direct Blue 1.

For dyeing tightly packed synthetic fibres such as PET and acetate rayon, disperse dyes are required. They are insoluble in water and the dyeing process involves the material being placed in a very fine, hot suspension of the dye with a chemical called a carrier. The carrier, an example being benzyl alcohol, transports the dye into the fibre when hot as the pores have expanded. Then, upon cooling, the dye becomes trapped. As the dye is insoluble and the fibre tightly packed, this dyeing method creates materials with excellent wash-fastness. Disperse dyes must be relatively small to enter the fibre.

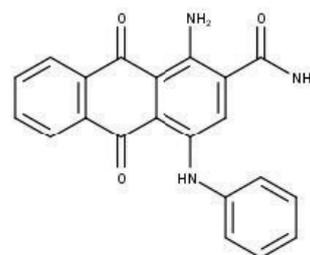


Figure 64 - The structure of Disperse Blue 6.

Vat dyeing is used to apply insoluble dyes to fibres. First, a reduced form of the dye that is itself soluble in water is applied to the material. Then, the dye is oxidised within the fibre, usually in air, into its original, insoluble form. Because of the insolubility of vat dyes, they often have very good wash-fastness. Indigo is a common example of a vat dye. Indigo itself is insoluble in water, but the reduced form, indigo white, is soluble.

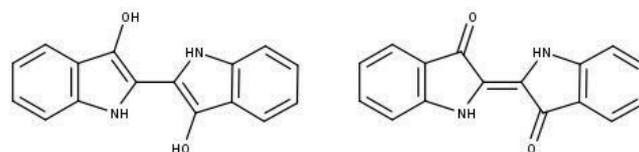


Figure 65 - The structures of Indigo White (left) and Indigo Dye (right).

Reactive dyes react with the fibre and so attach themselves via covalent bonds. They are usually used to dye plant-based fibres as they can react with the -OH groups of cellulose. The most common reactive

dyes are those based on haloheterocycles, heterocycles with attached halogens, and vinyl sulfones, sulfonyl groups next to double bonds. The haloheterocycles are reacted with cellulose in basic conditions. A deprotonated -OH group from cellulose attacks the heterocycle in a nucleophilic aromatic substitution. The vinyl sulfones are formed by elimination and go on to react with cellulose in basic conditions. A deprotonated -OH group from cellulose attacks the end carbon in a mechanism called Michael addition.

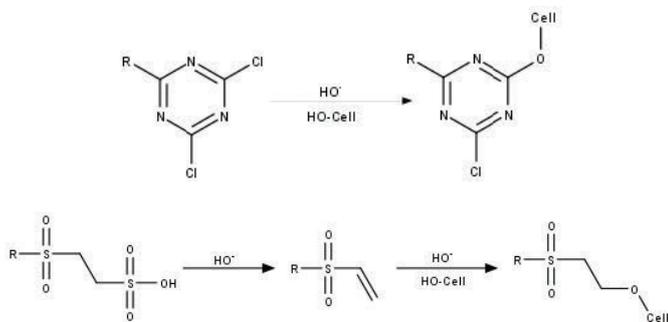


Figure 66 - Example reactions of a haloheterocycle (top) and vinyl sulfone (bottom) with cellulose, denoted Cell.

Azo dyes are synthesised by reacting a diazonium salt with a coupling component. To apply azo dyes, a material can be treated with a solution of the coupling component and then placed in a solution of the diazonium salt, forming the dye on the fabric, or vice versa.

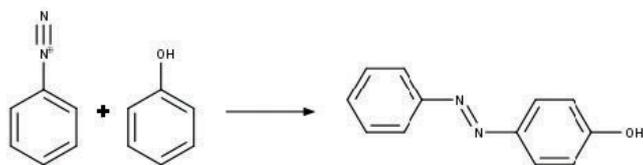


Figure 67 - Example of an azo coupling reaction.

7.1.3 Mordants

It is often the case that the dye alone cannot form strong enough interactions with the fibre and so has poor fastness. This is often the case with direct dyes. To solve this issue mordants can be used. A mordant is a substance that helps fix a dye to a material, and dyes that require mordants are called mordant dyes.

Mordants are usually inorganic metal salts containing a metal ion with an oxidation state of at least +2, often aluminium or iron(III). A common example is alum, $KAl(SO_4)_2 \cdot 12H_2O$. The metal ion can attach to the dye via both a covalent and a coordinate bond in a process known as chelation.

When a mordant dye and metal ion chelate together, the complex formed is called a lake. Generally, the covalent bond is to an -OH oxygen and the coordinate bond to a -C=O oxygen.

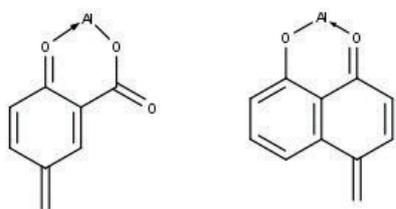


Figure 68 - Two examples of metal-dye lakes.

The metal can attach to more than one dye molecule, and this does happen. However, not all of the metal ions form complete complexes with the dye, as some of them form a complex with the fibre too. In this way the dye is attached to the fibre through the metal ion.

Mordants can also alter the colours of dyes due to the presence of the metal in the conjugated system. This is because the orbitals on the metal can affect the energy difference between the HOMO and the LUMO.

Cellulose-based materials do not bond well to mordant dyes as they are unable to form chelations with the metal ions. Mordant dyes are normally used to dye protein-based substances. In proteins, there are often many hydroxyl and carboxyl groups available, with which the metal can chelate, creating a dye-metal-fibre complex.

7.2 BLEACHING

7.2.1 Bleaching Mechanism

Bleaching a material is done by destroying the chromophore of the dye. Chemical bleaches react with the chromophore and either remove double bonds from it or break it apart completely. This interrupts the conjugated system, meaning the dye can no longer absorb visible light, making it colourless.

Most bleaches are strong oxidising agents which can break bonds in several different ways. Some are reducing agents which can convert double bonds into single bonds. It is also possible to cleave bonds simply using energy, so heat and light of high enough energy such as UV light, can bleach materials.

As a result of their ability to cleave bonds and destroy certain molecules, bleaches are highly effective at denaturing proteins. This makes them dangerous to humans, but also makes them very good disinfectants as they can easily kill bacteria.

7.2.2 Common Bleaches

Some of the most common bleaching agents are those based on chlorine. The first chemical bleach was chlorine gas and since then several other bleaches containing chlorine have been discovered. Chlorine itself is mostly used for disinfecting water but can be used to bleach wood pulp. Sodium hypochlorite, $NaClO$, is often simply called bleach and is generally used in households. A mixture of calcium hypochlorite, $Ca(ClO)_2$, calcium hydroxide, $Ca(OH)_2$, and calcium chloride, $CaCl_2$, creates bleaching powder, which has many of the same uses as sodium hypochlorite.

An example of sodium hypochlorite acting as a bleach is its reaction with an alkene. The chlorine atom in the ClO^- ion has a partial positive charge and can act as an electrophile. The double bond attacks this atom, forming a three-membered ring as an intermediate, which is then attacked by the solvent, water, forming a halohydrin, which can undergo further reactions. The result is that the double bond has been broken.

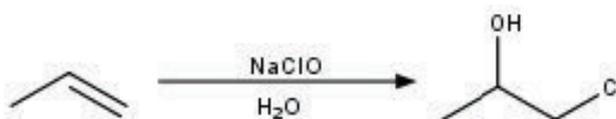


Figure 69 - Reaction of sodium hypochlorite with an alkene.

The other most common bleaches are those based on peroxides. These are characterised by an O-O peroxide bond which is easily broken, producing highly reactive species. Hydrogen peroxide, H_2O_2 , is used to bleach wood pulp and hair and can be used to prepare other bleaching agents. Sodium percarbonate, Na_2CO_3 , and sodium perborate, $Na_2H_4B_2O_8$, are other examples of peroxide bleaches and have a wide range of uses.

SECTION 8 SPECIFIC EXAMPLES

8.1 IMPORTANT EXAMPLES IN LIVING ORGANISMS

8.1.1 Chlorophyll

Chlorophyll is the green pigment found in plants, algae, and any other living organism that photosynthesises. Its function is as a photoreceptor, meaning it traps light. This light then catalyses the production of glucose via photosynthesis. The ability of chlorophyll to absorb light is very closely related to the theory of dyes we have covered.

Chlorophyll, like any other dye, contains a large conjugated system. The chromophore is a substituted porphyrin ring chelated with a central metal ion of magnesium. The structures of the two main types of chlorophyll, A and B, are shown below. The only difference is that in chlorophyll A, the R group is $-CH_3$, and in chlorophyll B, it is $-CHO$.

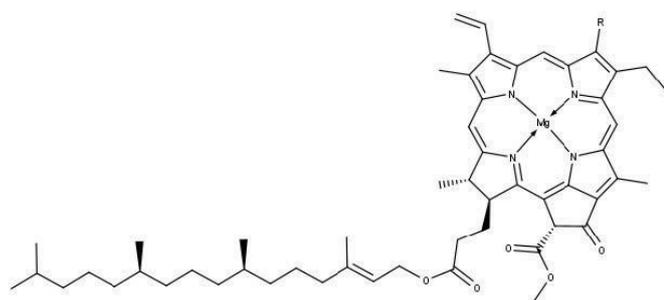


Figure 70 - The structure of chlorophyll.

The extended conjugated system is clear, stretching over the porphyrin and some of the attached groups. The wavelength of light absorbed is further altered by the magnesium, whose orbitals can interact with those of the conjugated system.

Chlorophyll A and B work together in plants to absorb a large range of the visible spectrum, allowing sunlight to be used as a source of energy. Wavelengths that one type fails to absorb are often made up for by the other. However, there is still a gap in the absorbance spectrum from 500nm to 600nm, which corresponds to green light, causing the green colour of chlorophyll.

In photosynthesis, energy from sunlight is absorbed by the conjugated system, leading to the excitation of an electron in chlorophyll. This electron can now be easily transferred to other molecules and a long chain of electron transfers leads to the transfer of an electron to a CO_2 molecule, reducing it, and the removal of an electron from H_2O molecule. Chlorophyll is bound to the back of a large, complex protein which positions it perfectly to react with any nearby water and carbon dioxide quickly and efficiently.

As chlorophyll has such a strong absorbance in the visible spectrum, it

masks the colours of other molecules present in leaves. This can be seen in autumn when the chlorophyll decays, allowing the oranges and reds of carotenoids to be seen. Also, when leaves are cooked, they become slightly more yellow as the magnesium is removed from the chlorophyll molecules.

8.1.2 Retinal

Retinal is found in the eye and is a molecule that allows humans to see. It undergoes a cycle of chemical changes, together with the protein opsin, called the visual cycle. The retinal molecule contains an extended conjugated system. The structure of this conjugated system is why we see the wavelengths of light that we do, and not, for example, ultraviolet light.

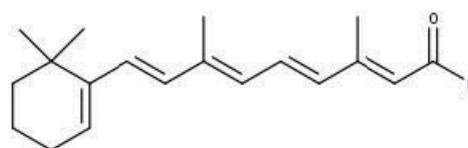


Figure 71 - The structure of all-trans-retinal.

Retinal is very similar in structure to β -carotene. As humans cannot synthesise retinal, we must ingest β -carotene through foods such as carrots, which can then be cleaved to give vitamin A (retinol) and through oxidation, retinal.

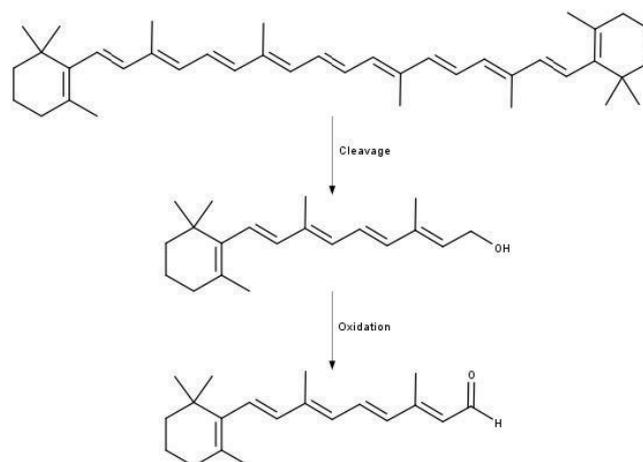


Figure 72 - A summary of the conversion of β -carotene to all-trans-retinal.

At a certain point in the visual cycle, a molecule of 11-cis-retinal binds to the protein opsin via a lysine residue. This new retinal-opsin molecule is called rhodopsin and has a strong absorbance in the region of 400 nm–700 nm, depending on the type of opsin. When a photon of the right wavelength is absorbed by the rhodopsin, the energy goes converts the double bond between the 11th and 12th carbon into a single bond, meaning it is free to rotate. When it has rotated through 180° , the double bond reforms, now in a trans configuration. The retinal is now all-trans-retinal, which does not fit the opsin binding site well, so the link between the retinal and the opsin weakens, and several fast reactions occur before they detach completely. This sudden movement is transferred through the protein to the membrane it is attached to, and eventually is picked up by nerve cells in the optic nerve which send a signal to the brain. The brain detects these and so we can see. The all-trans-retinal can undergo a series of enzyme-catalysed changes to reform 11-cis-retinal and the cycle repeats.

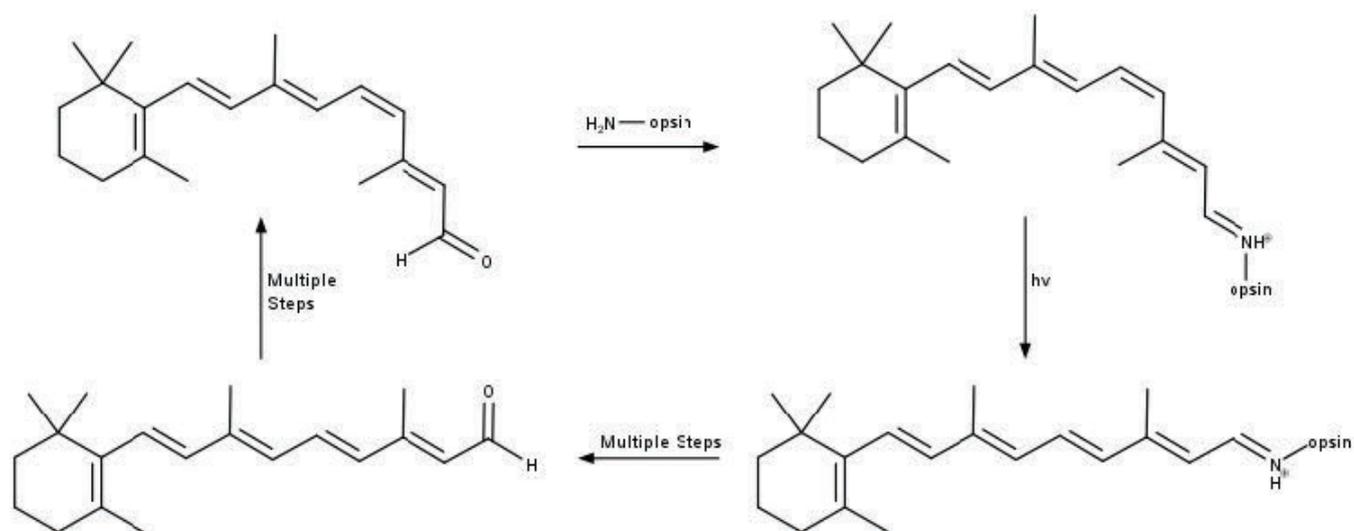


Figure 73 - A simplified diagram of the visual cycle. 11-cis-retinal (top left) is converted into rhodopsin (top right), then straightened (bottom right), then cleaved to all-trans-retinal (bottom left) and then converted back into 11-cis retinal.

There are three types of rhodopsin, each with a slightly different structure, that absorb at different wavelengths. The three are responsible for light in the red, green, and blue portions of the visible spectrum and all three working together results in our ability to see the colours that we do.

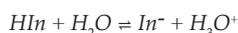
8.2 PH INDICATORS

8.2.1 General Mechanism

Certain chemicals appear different colours in acidic and basic conditions and can, therefore, be used as pH indicators. The pH of a solution is defined as the negative logarithm, base ten, of the concentration of H₃O⁺ ions.

$$pH = -\log_{10}[H_3O^+]$$

The colour change is usually caused by the dissociation of an H⁺ ion from the indicator. The neutral, *HIn*, and deprotonated, *In*⁻, forms of the indicator are in equilibrium with each other.



The equilibrium constant for this reaction is called the acid dissociation constant, *K_a*. Another constant, the *pK_a*, is defined as the negative logarithm, base ten, of the acid dissociation constant. The *pK_a* values of different indicators can be found in data books.

$$K_a = \frac{[H_3O^+][In^-]}{[HIn]}, \quad pK_a = \log_{10} K_a$$

There is an equation linking the concentration of *HIn* and *In*⁻, the pH of the solution and the *pK_a* of the indicator (the *pK_{in}*) called the Henderson-Hasselbalch equation. It can be derived by taking logarithms of both sides of the *K_a* equation.

$$pH = pK_a + \log_{10} \frac{[In^-]}{[HIn]}$$

From this equation, it can be deduced that if the pH is equal to *pK_{in}*, the concentration of *In*⁻ is equal to the concentration of *HIn*. If the pH is below *pK_{in}*, the concentration of *In*⁻ is less than that of *HIn*. If the pH is above *pK_{in}*, the concentration of *In*⁻ is greater than that of *HIn*.

For a weak acid indicator where *HIn* has a colour, say red, and *In*⁻ a different colour, say blue, then the colour changes can be estimated. At a pH equal to *pK_{in}*, the concentrations of *HIn* and *In*⁻ are equal, so the solution is purple. At a lower pH, the concentration of *In*⁻ is smaller than the concentration of *HIn*. As the pH scale is logarithmic, after about one unit of pH, the concentration of *HIn* is already about ten times larger than that of *In*⁻, so the solution is red. At a higher pH than *pK_{in}*, the concentration of *HIn* is smaller than the concentration of *In*⁻, so the solution is blue.

For any pH indicator, there is a *pK_{in}* and a range either side of this in which the solution is undergoing a colour change. The best indicators have a clear colour change and a small range over which the colour is changing.

8.2.2 Common Examples and Acid-Base Titrations

A universal indicator gives an approximate measure of pH by having a wide range of colours in different pH values. Universal indicators are composed of a mixture of several indicators, each specifically selected for their *pK_{in}* and colour change. When the correct indicators are mixed, a solution can be created that steadily changes through multiple different colours as the pH is altered, which is very useful for qualitative analysis.

The most common universal indicator is composed of a mixture of thymol blue, methyl orange, methyl red, bromothymol blue and phenolphthalein. This mixture results in a colour change from red in strong acid to violet in strong alkali, following the visible spectrum.

Indicators are often used in acid-base titrations, and the two most common indicators for this are phenolphthalein and methyl orange. Phenolphthalein loses two protons between pH 8.2 and 10.0, going from the colourless *H₂In* to the bright pink *In*²⁻ in this range. Methyl orange changes between pH 3.2 and pH 4.4 from the red zwitterion, *HIn*, to the yellow *In*⁻.

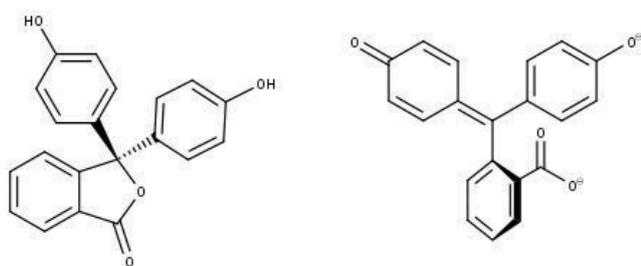


Figure 74 - The structures of phenolphthalein below pH 8.2 (left) and above pH 10.0 (right).

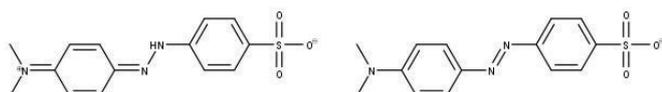


Figure 75 - The structures of methyl orange below pH 3.2 (left) and above pH 4.4 (right).

When choosing an indicator for a titration, it must change colour at a pH near the equivalence point, the point where the two substances have been mixed in equal proportions. The shape of the titration curve allows for a large variation in pH from the equivalence point with minimal loss of accuracy. For this reason, both phenolphthalein and methyl orange change colour close enough to pH 7 that they can be used for strong acid-strong base titrations. But for weak acid-strong base titrations, the equivalence point is at a higher pH, so methyl orange is no longer a valid indicator to use. The opposite is true for strong acid-weak base titrations, so phenolphthalein is not valid. For weak acid-weak base titrations, the shape of the titration curve is such that neither of these indicators are useful.

SECTION 9 CONCLUDING REMARKS

This exploration of the chemistry of dyes has taken us through many branches of chemistry from quantum mechanics and atomic and molecular orbitals to biochemistry and acid-base indicators. It is clear that the study of dyes is a rich field full of interest and that there is a lot to be gained from studying them.

Dyes not only hold an important place in chemistry but also our lives. All the clothes we wear every day have most likely been dyed or bleached in some way. Then there is the fabric on the furniture, the food dyes in the cupboard, the list goes on. Even outside, away from man-made objects, the landscape is filled with the vibrant colours of plant life. It is impossible to escape the importance of dyes in our daily lives.

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