NGEE ANN SCHOOL OF ENGINEERING

22 WEEKS INDUSTRY INTERNSHIP

WITH

A*STAR Institute of Chemical and Engineering Sciences (ICES)

FINAL REPORT

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Declaration by student:

1. By submitting this report online, I confirm that the report has been submitted to and vetted by my company supervisor, and thereby confirm that the report contains no confidential material from the company.

2. I declare that the report is written by me and not plagiarised from other sources.

Dr. Liu Yan_____29/07/2021 Alyssa Png 09/08/2021

Supervisor Name/Signature/Date Student Signature/Date

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LIST OF ABBREVIATIONS

Abbrevation	*Explanation*
*A*STAR*	Agency for Science, Technology, and Research
DI	Deionised
DRIFTS	Diffuse Reflectance Infrared Fourier-Transform Spectroscopy
FTIR	Fourier-transformed Infrared Spectroscopy
GC	Gas Chromatography
ICES	Institute of Chemical and Engineering Sciences
ICP-OES	Inductively coupled plasma-optical emission spectrometry
IR	Infrared
JSON	JavaScript Object Notation
K-M	Kubelka Munk
MCT	Mercury-Cadmium-Telluride
MFC	Mass Flow Controller
MW	Molecular Weight
NMR	Nuclear Magnetic Resonance
NSTB	National Science and Technology Board
R&D	Research and Development
RBF	Round Bottom Flask
RE	Rotary Evaporation
SEM	Scanning Electron Microscope
TEM	Transmission Electron Microscope
XRD	X-ray Diffraction
XRF	X-Ray Fluorescence

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Summary

This report consists of the work done during my internship with the Agency for Science, Technology, and Research (A*STAR) from 8 March 2021 to 6 August 2021. A*STAR is Singapore's lead public sector research and development (R&D) agency. With the help of the wider research community as well as other public sector agencies, A*STAR aims to achieve its mission to advance science and develop innovative technology to further grow the economy as well as improve lives.

I have the privilege of working under the Institute of Chemical and Engineering Sciences (ICES). Due to the growth of the pharmaceutical industry in recent years, the contribution of chemistry and chemical engineering science to Singapore's economy has significantly risen. In hopes to strengthen the local science and technology base, ICES was set up to provide well-trained R&D manpower, create a secure science base and enhance technology and infrastructure.

Before my internship, I set out the following learning goals for myself to achieve:

1. To gain new knowledge and exposure to the research industry
2. To enhance and improve my communication and brainstorming skills
3. To learn the roles and responsibilities of a being researcher
4. To work well and forge a strong relationship with my co-workers

In this report, I would focus on the overview of A*STAR and ICES as well as the various tasks I was assigned throughout my 22 weeks. My task includes conducting experiments for the assignment project on Catalytic Conversion of Carbon Dioxide (CO2) to value-added products, plotting graphs, and analysing data.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Acknowledgement

My experience interning under the Institute of Chemical and Engineering Sciences (ICES) for the past 22 weeks has been very eye-opening and rewarding. I would like to express my gratitude to both Ngee Ann Polytechnic and A*STAR for this opportunity to learn new things and gain real-world work experience in the Research Industry.

A special thank you to Dr. Liu Yan, my company supervisor, for her constant encouragement and guidance throughout the 22 weeks. Despite her busy schedule, she never fails to check up on my progress and takes the time to read and provide useful knowledge to improve my weekly reports. Knowing that I have little chemistry background, she has always reassured me and provided me with useful reading materials to boost my understanding of my assigned project.

Xiao Xin, my student buddy at ICES, is someone who has given me a lot of guidance and help. He has provided an environment for me to not be afraid to ask questions and learn many new things. I really appreciate all the time and effort he has put in to ensure that my internship is so fruitful and enriching. Not only does he take his time to teach me how to use the instruments in the lab, but also explains to me the science behind such instruments.

Another person I would like to thank is Dr. Abdiel Foo, my NPIS mentor, for helping me arrange this internship. I am very grateful for his willingness to help clear my doubts and providing constant guidance and support.

Finally, I would also like to thank all the wonderful colleagues at ICES for being so welcoming and helpful towards me throughout the past 22 weeks. It was a great privilege to be able to work alongside such professional and inspiring researchers.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

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Chapter 1. Introduction

1.1 A*STAR

The Agency for Science, Technology and Research (A*STAR) is Singapore's lead public sector R&D agency. A*STAR plays an important role in building up talent and leaders for their Research Institutes, the wider research community, and industry. Being a science and technology organisation, A*STAR aims to bridge the gap between academia and industry in terms of research and development.

1.1.1 Company Logo

*Figure 1-1: A*STAR Logo*

*(A*STAR, n.d.)*

1.1.2 History

The origins of A*STAR can be traced back to 30 October 1967, when the Science Council of Singapore was officially set up to develop the nation's scientific and technological capabilities. Initially created to mainly provide advice, their work consists of writing reports and recommendations regarding research and development (R&D) for the then Ministry of Science and Technology. On 11 January 1991, the Science Council was upgraded to a statutory board known as the National Science and Technology Board (NSTB). Philip Yeo became the chairman of NSTB in August 2000. The organisation was then split into two research groups. One focusing on science and engineering while the other on the biomedical field. This reorganisation helped to better direct the company's resources by bringing together previously disparate R&D-related organisations under one umbrella. It also brought about more attention to the need for manpower in the science and technology fields. In January 2002, NSTB was renamed (Moasi, 2019).

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1.1.3 Mission

A*STAR's mission is to advance science and develop innovative technology to further grow the economy as well as improve lives. This helps to promote mission-oriented driven research that advances scientific discovery and technological innovation. Collaboration with the wider research community as well as other public sector agencies will lead to meaningful and impactful results. To enhance the lives in Singapore, A*STAR also focuses on contributing to societal benefits such as improving outcomes in healthcare, urban living, and sustainability.

The organisation aims to achieve this mission by combining its capabilities with Multi-National Corporations and Globally Competitive Companies to bring about change. A*STAR is also working alongside Local Enterprises for productivity and gearing them for growth. R&D-driven start-ups supported by A*STAR will be better prepared to tackle unexcepted outcomes and better shaped for success. Through this, the organisation will be equipped with the necessary manpower to improve the science and technology sectors, guide and manage R&D initiatives and monetise R&D results. This will help to push for innovation and enhancement of the nation's knowledge-based economy (A*STAR, n.d.) .

1.1.4 Vision

A*STAR's vision is to become a worldwide leader in science, technology, and open innovation. It is a catalyst, enabler, and convenor of significant research efforts for both within and beyond the research community in Singapore. With open innovation, the organisation can collaborate with both its public and private partners to achieve a better economy and society using science and technology (A*STAR, n.d.).

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

1.1.5 Organisation Chart

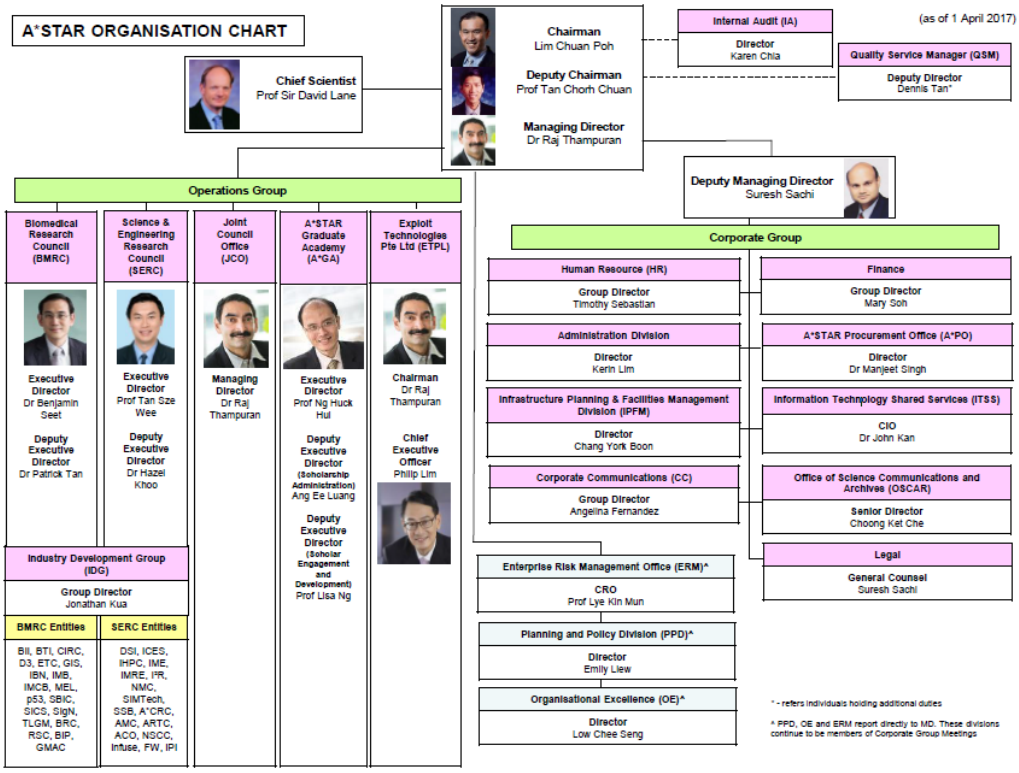

Figure 1-2: Organisation Chart

1.2 Institute of Chemical and Engineering Sciences (ICES)

Singapore is a major oil refining centre with a long history and is strategically located at the heart of Asia. Therefore, the chemical industry plays a huge role in the Singapore economy for many years. With the growth of the pharmaceutical industry in recent years, the contribution of chemistry and chemical engineering science to Singapore's economy has significantly risen.

To secure this position and foster future development to grow from a manufacturing dependency to a more knowledge-based dependency, A*STAR has initiated more high-tech research and development based on the business environment. In hopes to strengthen the local science and technology base, A*STAR and Economic Development Board (EDB) has established the Institute of Chemical and Engineering Sciences (ICES) to provide well-trained R&D manpower, create a secure science base and enhance technology and infrastructure to aid future growth.

ICES was once a small centre in the National University of Singapore (NUS) set up as an autonomous national research institute under A*STAR on 1 October 2002.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Since then, the institute has expanded and now consists of elite laboratories, pilot facilities, and the necessary infrastructure to carry out world-class research programs in chemistry and chemical engineering sciences. From exploratory research to process development, optimisation and problem-solving, ICES can cover a range of activities (A*STAR, n.d.).

1.2.1 ICES Logo

Figure 1-3: ICES Logo

(Asia Research News, n.d.)

1.2.2 Organisation Chart

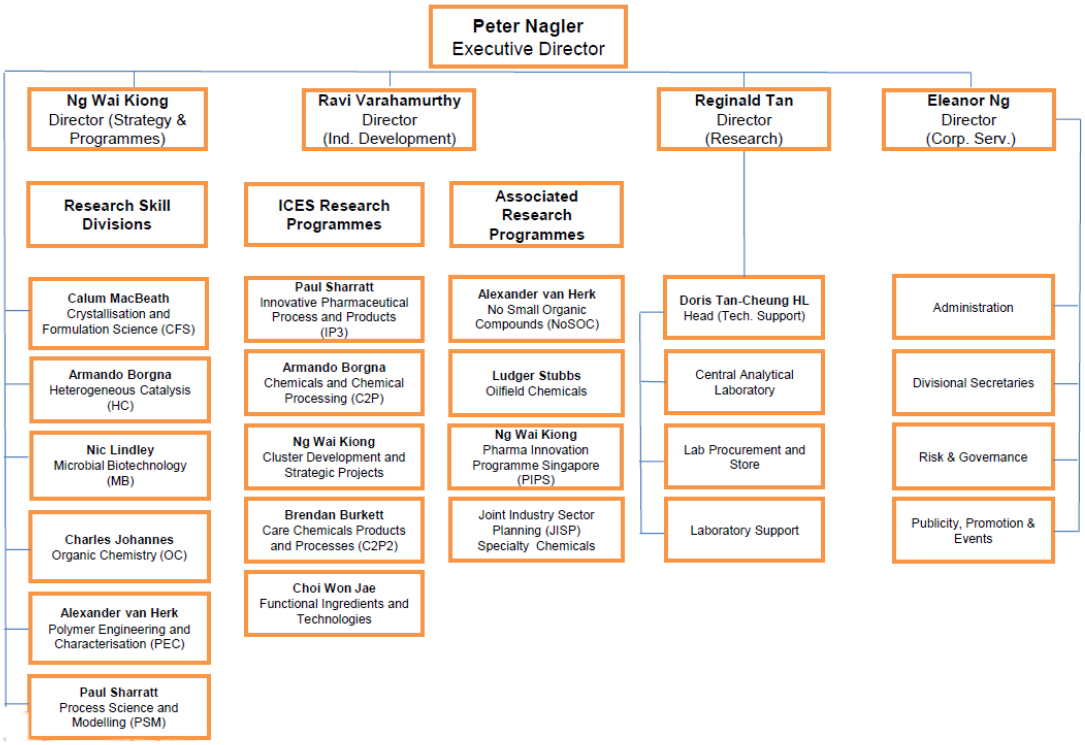

Figure 1-4: ICES Organisation Chart

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1.3 Process and Catalysis Research

The Process & Catalysis Research division consists of four teams that cover the spectrum of design and synthesis, development and scale-up, and process of homogeneous and heterogeneous catalysts. The first team, Process R&D, tackles solutions for more sustainable and cost-effective process design, innovation and scale-up for speciality chemicals and pharma. Secondly, the Decarbonising Strategy team comes up with sustainable catalysts and processes to better aid carbon capture, utilisation and storage activities. The next team, the Heterogeneous Catalysis team, focuses on the design and synthesis of future generation heterogeneous catalysts and improved and novel catalysts. Lastly, the Homogeneous Catalysis team specialises in coming up with designs and developing ligands and homogeneous catalysts for speciality chemicals and pharma (A*STAR, n.d.).

1.4 Roles and Responsibilities

My task as an intern was to help assist with conducting experiments under the Catalytic Conversion of Carbon Dioxide (CO2) to value-added products project. These experiments include working with various instruments and preparing different catalysts.

For most of the internship, I worked with a Fourier-transformed Infrared Spectrometer (FTIR) to conduct Diffuse Reflectance Infrared Fourier-Transform Spectroscopy (DRIFTS) experiments on various catalysts. The experiments were split up into two separate procedures, stepwise and mixed gas. Upon the completion of each experiment, the experimental data was plotted and analysed using Excel and Origin.

Besides DRIFTS, I had to learn the different preparation, collection and testing techniques used for catalysts. This involves the mixing of different reactants under different environments to obtain high-performance catalysts needed for the project. These experiments will be further elaborated on in the following chapters.

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Chapter 2. Main project

Diffuse Reflectance Infrared Fourier-Transform Spectroscopy (DRIFTS)

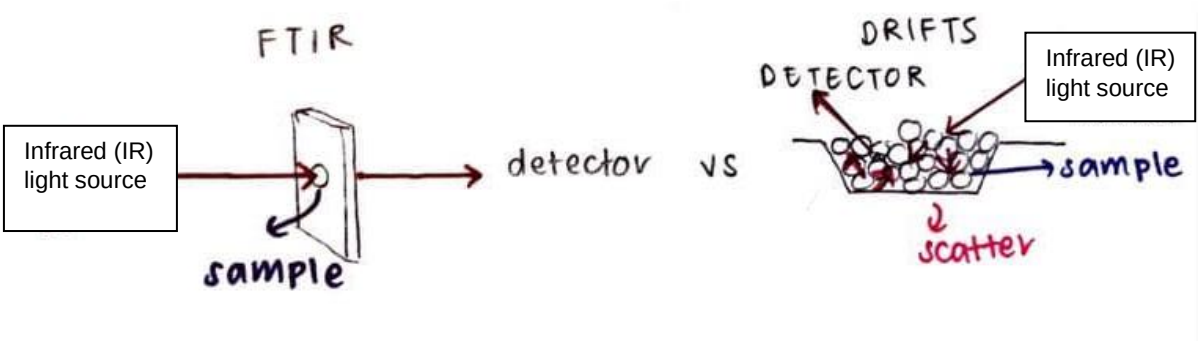

Figure 2-1: FTIR vs DRIFTS

Fourier-transformed Infrared Spectroscopy (FTIR) is a method used to measure the infrared spectrum of absorption and emission of a sample. Whereas Diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) is a type of FTIR technique that results from the incident radiation penetrating the particles leading to a subsequent scatter from the sample matrix. Although both use similar concepts, their functions are different. FTIR is used to detect the amount of light absorbed by the sample while DRIFTS is used to analyse the shape and the reflectivity of the sample. Both analyses are measured at a range of wavelengths within the infrared (IR) region. The IR ray shone onto a sample will interact with the particles and reflect off their surfaces. This causes the light to be diffuse and scatter throughout the sample. Refer to Appendix A1 for experiment setup.

2.1 Pre-treatment

Before the actual experiment, the sample was put under reduction in an external horizontal tube furnace. The reason for this was that the temperature at which this reduction takes place exceeds the maximum temperature the DRIFTS chamber can withstand. After reduction, the sample was taken out of the furnace and grounded using a mortar and pestle. Reduction is an important method to remove any impurities found in the sample. The presence of such impurities can affect the

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accuracy of the experimental results as they will alter the way the sample interact with the IR ray.

For all DRIFTS experiments conducted, 50mg of KBr was grounded using a mortar and pestle and loaded into the chamber before the powdered sample. The reason for grounding the KBr and sample is to ensure uniform particle size throughout for even diffuse reflectance.

The chamber was then closed, and the temperature was increased to 300°C. Hydrogen was then purged into the chamber to allow the sample to undergo further reduction for 30 minutes. Further reduction is necessary to get rid of any impurities that may have formed while the sample was exposed to the atmospheric air. The oxygen found in the atmospheric air will oxidise the sample forming impurities on its surfaces. After 30minutes, helium, an inert gas, was purged into the chamber to get rid of the leftover hydrogen in the chamber. The liquid N2 was then topped up and the software was turned on.

The background spectrum was then taken as a reference used to observe any new peaks in the spectra taken throughout the experiment. This was an important step to ensure that the data obtained at the end of the experiment was based on the sample alone and not due to the other chemicals such as gaseous chemicals that are always present within the chamber.

2.2 Procedures

Through researching and trying out various trial experiments, the two standardised procedures, stepwise and mixed gas, were decided. The process of how each procedure came about will be further elaborated in the paragraphs below.
Initially, for the stepwise procedure, pure gas reactant B was not pulsed but purged into the chamber for 2 minutes. Helium was then purged into the chamber for another 2 minutes for desorption. Desorption involves the removal of any physically absorbed substances. During these 2 minutes, the desorption spectra were taken. This procedure, involving absorption followed by desorption, was repeated until the spectra had stabilised. The stability of spectra will be explained under section 2.4.4 “Data analysis”. Due to the absence of any clear or distinct changes between the

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peaks on the spectra, this procedure was rejected. In hopes to observe a better transition of reactions, the spectra were also taken during the purging of gas reactant B. This was because the reaction was mainly taking place during the absorption of gas reactant B. Although, there were more distinct changes in the spectra, it was not observed consistently throughout all the experiments. With the help of reference literature, it was decided to reduce the purge duration of gas reactant B to 10 seconds. This was done in hopes to slow down the rate of reaction and therefore, see a better breakdown of the transformation of reactions. This was known as pulsing. To promote a more effective reaction, a small percentage of gas reactant A, which was diluted with Helium, was purged continuously into the chamber. This process helped to obtain stepwise procedure 1 which was conducted for the first 11 weeks of the internship. A second stepwise procedure was formed later in the internship when a certain type of catalyst was introduced. After looking at various research papers, it was decided that gas reactant B was to be purged continuously instead of pulsed while the absorption peaks were taken. This process will better suit the characteristic of the new catalyst.

The mixed gas procedure was then generated to observe all the changes occurring on the surface of the sample during the whole reaction, from reacting gas reactants A and B to obtaining the finalised products.

2.2.1 Stepwise

After the background spectrum was taken, gas reactant A was purged into the chamber for the sample to undergo absorption. Two DRIFTS spectra were taken, one after 30 minutes and the other after 32 minutes under absorption. If there were no changes between the two spectra, the desorption of gas reactant A could begin. This involved purging Helium into the chamber to get rid of any physically absorbed gas reactant A. An FTIR spectrum was scanned every 5 minutes until 30 minutes had passed.

<u>Procedure 1 (pulsing):</u>

To observe the transformation of reaction that intermediates on the sample surface, gas reactant B was pulsed into the chamber. Meanwhile, a gas mixture of Helium and gas reactant A was purged continuously into the chamber. Gas reactant B was

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pulsed for 10 seconds, before helium was purged into the chamber for desorption for 2mins. During desorption, a spectrum was taken from 0 to 20, 20 to 40, 40 to 80 and 80 to 120 seconds. This was repeated until the spectra obtained have stabilised, usually after 8 pulses.

Procedure 2 (continuous flow):

Once the desorption spectra were taken, the sample was left under a continuous flow of gas reactant B. During the first 2 minutes of absorption, three spectra were taken every 40 seconds. After the first 2 minutes, a spectrum was taken at 2 minutes intervals until the absorption duration was 30 minutes.

2.2.2 Mixed Gas

Unlike the stepwise experiment, a gas mixture of both gas reactants was purged into the chamber for 30 minutes for the sample to undergo absorption. For the first 2 minutes, a spectrum was taken from 0 to 20, 20 to 40, 40 to 80 and 80 to 120 seconds. The first 2 minutes of purging the gas mixture are very crucial when observing any intermediates as it is when the rate of reaction was the highest. After the first 2 minutes, a spectrum was taken every 2 minutes until 30 minutes passed.

During the second half of the internship, the intervals for taking the first 2 minutes spectra were changed to 40 seconds. One spectrum was also taken every 3 minutes during the absorption period of 30 minutes. Refer to Appendix A3 for the plotting of DRIFTS spectra.

2.3 Data analysis

The main goal of this experiment was to observe the intermediate species of each reaction and to identify the products or intermediate species obtained from each sample. Spectra were deemed as stable when there were no more changes between the most recent spectrum and the one taken before it.

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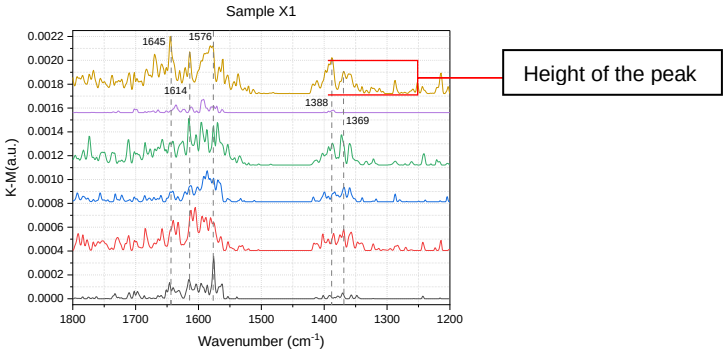

Figure 2-2: Pulse graph of Sample X1

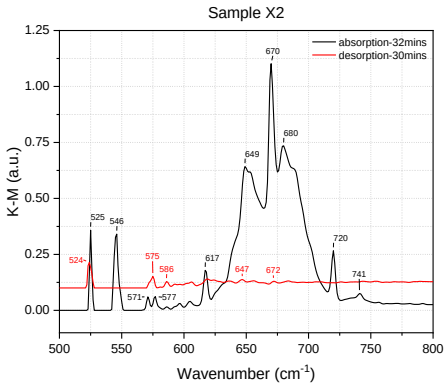

Figure 2-3: Absorption and Desorption graph of Sample X2

If the sample was too dark, the spectra obtained would be very noisy and the intensity of the peaks would be very low (height <0.01) as seen in Figure 2-2 and the desorption graph in Figure 2-3. When the sample is dark, the diffuse reflectance occurrence within the sample is low. Therefore, causing the reflected signal to be very weak. To prevent obtaining such a graph, more KBr can be used, or the composition of the sample can be altered. The reduction temperature can also be lowered as during reduction colour change may be observed.

When plotting the spectra on the graph it is important to label the various desired peaks. By identifying and labelling, the type of sample could be match to the species of products and intermediates produced during the experiment.

Using a reference table similar to the table below, the peaks on the spectra can be identified and differentiated by the species they represent based on the wavelength they appear at.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Table 1: Example of FTIR spectrum reference table

(Winter, n.d.)

IR Absorptions of Common Functional Groups		
Functional Group	***Absorption Location (cm^{-1})***	***Absorption Intensity***
Alkane (C–H)	2,850–2,975	Medium to strong
Alcohol (O–H)	3,400–3,700	Strong, broad
Alkene (C=C) (C=C–H)	1,640–1,680 3,020–3,100	Weak to medium Medium
Alkyne (C≡C) (C≡C–H)	 2,100–2,250 3,300	 Medium Strong
Nitrile (C≡N)	2,200–2,250	Medium
Aromatics	1,650–2,000	Weak
Amines (N–H)	3,300–3,350	Medium
Carbonyls (C=O) Aldehyde (CHO) Ketone (RCOR) Ester (RCOOR) Acid (RCOOH)	 1,720–1,740 1,715 1,735–1,750 1,700–1,725	Strong

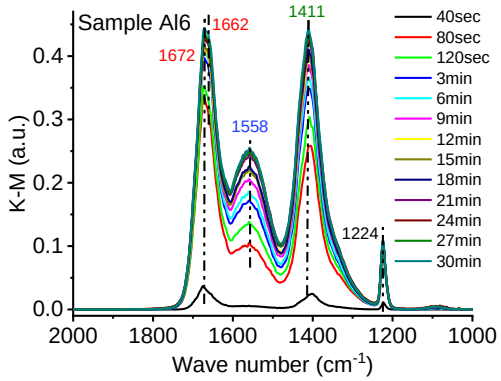

Figure 2-4: Sample Al6 spectra

For the project, the identification of the peaks was displayed using labels and dotted lines as seen in Figure 2-4. To differentiate between the species of products and intermediate, each species was represented by a colour. This was done on all the spectra of the different samples allowing better comparison between them.

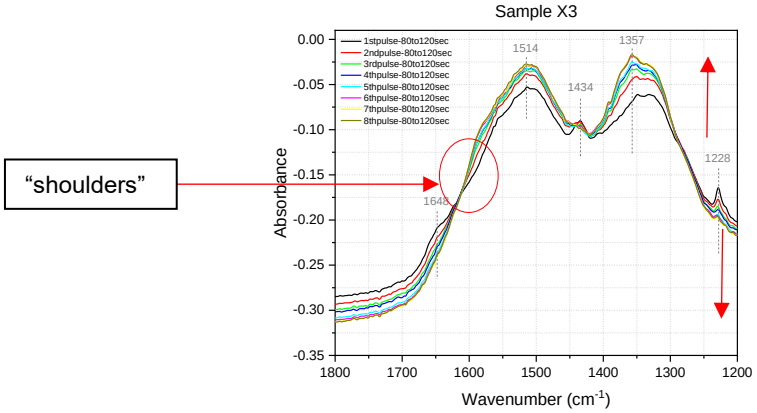

Figure 2-5: Pulse graph of sample X3

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

If a peak increased like the peak at 1357cm^{-1} in Figure 2-5, this indicated the formation of more of this product or intermediate species was being formed. If a peak decreased like the peak at 1228cm^{-1} in the above figure, this suggests that this peak represented an intermediate species that was being converted to a product. Therefore, the decrease in a peak may be the cause of an increase in a separate peak. It was very important to inspect the spectra carefully and thoroughly as even small peaks are valuable. Such small peaks may indicate the presence of a type of product and could be the reason behind the decrease in other peaks.

If a peak disappears faster than another peak, it may be because that specific material is less stable or more reactive to the gas reactant than the other. Another interesting analysis of the spectra observed was that a shift in a peak could be an indication of an addition or deletion of a new species of product to an existing species. Besides peaks, “shoulders” forming on the spectrum could suggest that a new peak was forming.

Samples containing one or more same elements may have similar spectra. Using these concepts, the accuracy of the experimental results could be determined. If the spectra obtained for a sample differs from that of other samples with a similar composition, it may suggest that the experimental results are incorrect. To test this hypothesis, the DRIFT experiment for this sample is conducted again. This will help to strengthen the credibility and accuracy of the research results.

2.4 Challenges Faced and Learning Points

With limited chemistry knowledge, I found it hard to understand the science concepts behind the experiment. Due to this, I was not confident enough to provide suggestions to better improve our results. Fortunately, when I did voice out my ideas, they were met by very supportive comments and constructive feedback from Xiao Xin. This encouraged me to continue to share my thoughts as well as ask questions when in doubt. As taught in school, I wanted to take more responsibility for my learning. I started researching more on DRIFTS and watching different YouTube videos. When I have a better understanding of the concepts behind the experiment, I will be able to provide more useful suggestions and play my part in improving the project’s experimental results. For example, when using low energy level (<70)

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

samples to carry out DRIFTS, the desired peak on the K-M spectra could not be observed. However, after doing some research, I brought up how some researchers use Absorbance to display their results. We soon realised that certain peaks could only be observed using Absorbance. This was because when using K-M in the presence of high-intensity peaks, like the gas-phase peak of the gas reactant A, smaller intensity desired peaks tend to be cancelled out. Therefore, it is evident that hard work pays off as I was able to further contribute to the project.

I would always be very paranoid about missing out certain steps since both procedures were quite lengthy. There was once that I had forgotten to open one of the valves controlling the flow of the gas reactant during the pre-treatment. Although this mistake only delayed the experiment, it was important to prevent this from happening again. Missing out steps can lead to worse consequences. Therefore, I wrote down the procedure in point form in my notebook so that I could run through the steps before each experiment. As I conducted the experiment, I would tick out each step ensuring that did not miss out on anything. I continued to do this until I was very familiar with the different procedures. It was very important for me to stay focus in the lab and to ensure not to be distracted when carrying out experiments.

Although it did not seem like a challenge at first, I soon realised the difficulty in finding the best way to display our experimental results. There were a lot of variations that we tested out, from labelling all the peaks to using shaded areas to section out the desired peaks. At one point, we also wanted to add a Z-axis (time) to display a three-dimensional spectrum of the whole experiment. However, this made the diagram was very messy and the spectra were overlapping. With the help and constant advice from Dr. Liu Yan, we were able to decide on our final designs. Through this process, I learnt the importance of the aesthetic of displaying any data. There are many ways of going about doing so but choosing the right one depends on the message we wish to convey. From the use of labels to setting the same X-axis range for all the spectra, there are many small details we could include to ease the analysis and comparison process. Data analysis is a skill that I will have to apply in the future. When I do encounter it, I will make sure to take note of how to properly plan out the aesthetic of my diagrams and apply the various tools I have learnt when working on this project.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

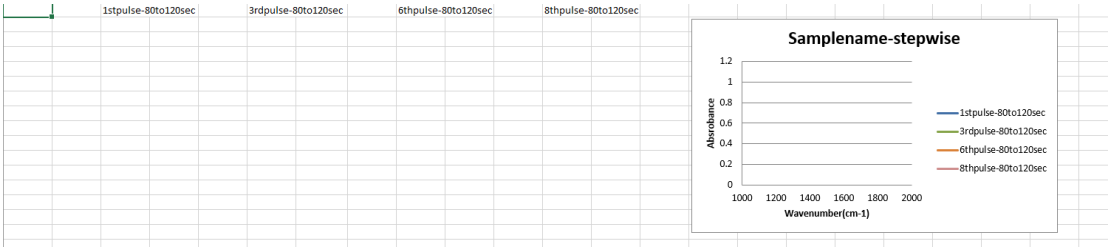

Figure 2-6: Example of stepwise template

At first, the plotting of data using Excel and Origin was quite challenging. Since there were quite a lot of data to handle all at once, making mistakes in transferring the data were bound to happen. In hopes to minimise this, I created templates as shown above for both procedures using Origin and Excel. Not only does this reduce the possibility of making errors, but it also helps to make plotting more efficient. We are taught as engineers the importance of efficiency and to make use of our skills to make a tedious task simpler. The energy and time saved from not doing repetitive tasks can be used doing other tasks. After setting up the templates, I was able to be more productive and plotting the spectra was more convenient. To save even more time, I decided to plot the spectra while conducting the experiment at the same time. By the end of the experiment, the graph had also been plotted. I was able to help Xiao Xin complete more tasks and observe him doing other kinds of experiments. Sooner or later, I was learning many new things at a faster pace than before.

As I join in for the project discussion, I was able to observe the team's interpersonal and communication skills. Although their views may be conflicting, they still listen attentively to each other's opinions and ideas before compromising on a unanimous solution. When Xiao Xin was explaining all the trial experiments for DRIFTS, the rest of the team was listening and only waited for Xiao Xin to finished before giving their inputs. Their occasional nods help to validate Xiao Xin's opinions. Likewise, as Dr. Liu Yan was giving her inputs Xiao Xin will be taking down notes. It was clear that to work as a team, there must be mutual respect formed between the teammates. With respect, effective communication will thrive, and constructive criticism can also be brought forward. All these are needed for the project to advance and to better our experimental results. Next semester, during my final year project, I hope that I will stay open-minded to my teammate's suggestions and gradually form a mutual respect for each other's ideas.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Chapter 3. Catalyst

Catalysts are foreign substances responsible for speeding up chemical reactions. Catalyst helps to convert reactants to products through a continuous and uninterrupted cycle of elementary steps. During these steps, the catalyst will transition into various reactive intermediates until it reaches the last step in which the catalyst regenerates back to its original form.

There are two main types of catalyst, Homogenous and Heterogenous. Homogenous catalysts are catalysts that share a common physical phase as that of the reactants or their solution form involved in the reaction. Heterogeneous catalysts are used in reactions with reactants of a separate physical phase than themselves.

One of the benefits of using industrial catalysts is to promote green catalytic processes. These are chemical processes that are altered to become more environmentally benign. They make use of the selectivity of catalysts to produce a high yield of the desired products while producing little to no unwanted side products. They are usually done under high energy efficiency.

3.1 Important concepts of a catalyst

3.1.1 The Sabatier Principle

The Sabatier principle acknowledges the existence of an intermediate compound formed between the catalyst's surface and at least one reactant. These intermediate species must be stable enough to be produced in sufficient quantities and labile enough to be converted into the final products or products. During the DRIFTS experiment, these intermediates are valuable indications of the different transitions of reactions occurring as the experiment is taking place. The presence of an unstable surface intermediate requires the chemical bonding between the reactant and the catalyst surface, more specifically their active sites.

3.1.2 Active Sites

Active sites can be determined as a combination of atoms that are unique to that of a catalyst. These active sites can vary from the case in which all the atoms are active to only a few being active. They are located at the exposed surfaces of catalyst which consist of multiple vacancies with sites that have different coordination

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numbers. The variation of coordination numbers will result in a variety of reactivities and activities corresponding to the various active sites.

3.2 Preparation of solutions

Figure 3-1: 100ml Volumetric flask

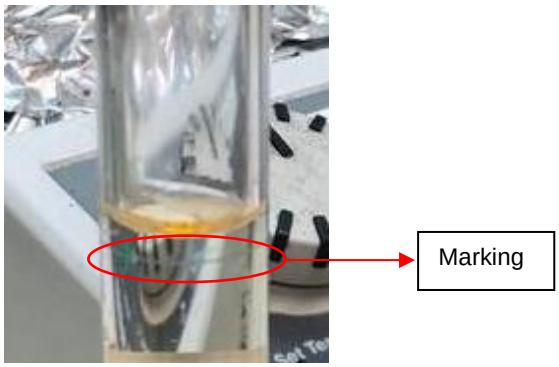

Figure 3-2: Marking on the volumetric flask

The solutions used for the preparation of a catalyst must be prepared beforehand. The solid reactants were first measured and dissolved in a beaker using a given volume of deionised (DI) water. This volume must be at most half of that of the volumetric flask used. The solution was then stirred until clear to ensure that all the solid reactants had completely dissolved. Once clear, the solution was poured into a volumetric flask and the beaker was rinsed 3 times with DI water. The diluted solution obtained after each rinse was poured into the flask. Using DI water, the flask was filled until the solution level reaches the marking on the flask as shown in Figure 3-2. This marking indicated that the desire solution volume was reached. The filled volumetric flask was stored until further use.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

3.3 Calculations

Various calculations had to be done to determine the mass or volume of the reactants needed to prepare the catalyst. The first step is to find the mole needed for each reactant, this can either be given or can be determined by the desired percentage or molar ratio of each component in the catalyst.

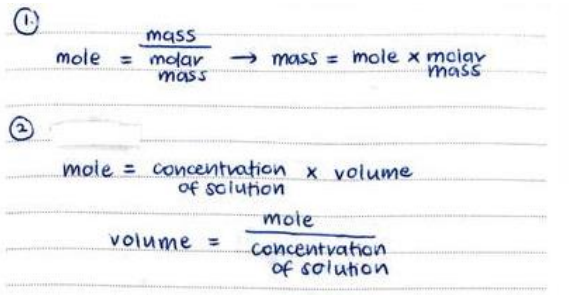

Figure 3-3: Mole Formulas

If the mole needed for each reactant was given, the formulas above can be used to find out the mass or the volume of the reactant needed. The molar mass, also known as molecular weight (MW) is a combination of all the individual atomic masses in a molecule. The MW is normally found written on the bottle of each reactant.

For preparing solutions, the volume of the solution and desired concentration of each reactant will be stated. When using a volumetric flask, the volume of the volumetric flask will be substituted as the volume of the solution. By having the value of both parameters, the mole of each reactant used can be calculated. Therefore, their desired mass can be found.

In the preparation of a catalyst, if the mole of each reactant is not provided, it can be calculated as seen in the figures below.

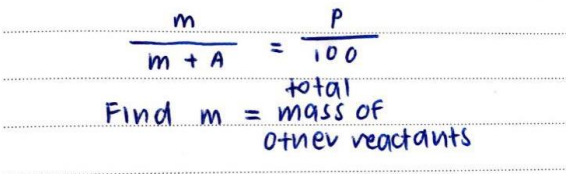

Figure 3-4: Step one, finding mass needed

Firstly, the mass of one of the reactants is fixed (A). Using the total percentage of the other reactant(s) (P), the combined mass (m) needed for the other reactants can be

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

found. If there was only one other reactant involved, the mass or volume needed for this second reactant can be found using the formulas in Figure 3-3.

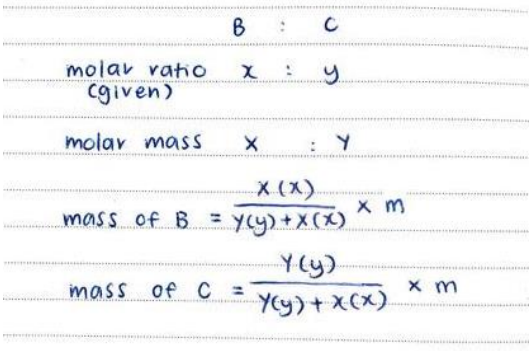

Figure 3-5: Finding the individual mass of each reactant

However, if there is more than one other reactant, the steps above can be followed to find the mass needed for each reactant. With the molar ratio and MW, the fraction of each reactant in terms of molar weight can be found. Using this fraction multiplied by the total mass of all the other reactants (m), the mass of each reactant needed can be found. If the volume is needed, the formulas in Figure 3-3 can be used by substituting in the appropriate mass, MW, and concentration.

To minimise calculation errors, an excel sheet was programmed. The first sheet was used to implement the formulas found in Figure 3-3. This was separated into 3 tables. One table was to calculate the mass of the solid reactant needed to prepare a solution while the other two were for the basic mole calculations used in catalyst preparation.

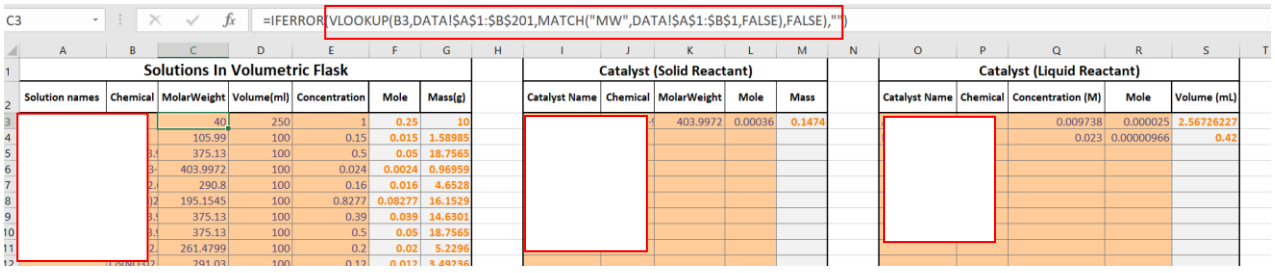

Figure 3-6: Example Basic Calculations

For columns B, D and J, the user can select from a list stored in a separate sheet, the “DATA” sheet as seen in Figure 3-7, using the data validation feature. This feature will prevent the user from keying in any invalid inputs. For column D, the volume of the volumetric flask was fixed to either 250ml or 100ml. After a chemical

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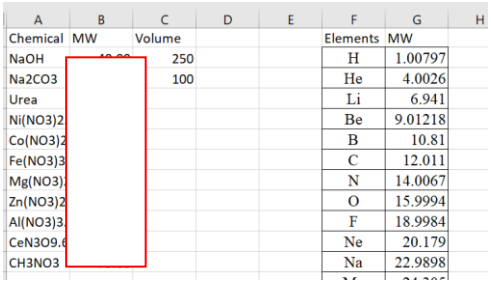
was selected for columns B and J, the MW will automatically be printed out. As seen in the figure above, the formula “MATCH()” was used to locate the heading number “MW” from column A to B in the “DATA” sheet. “VLOOKUP()” was then used to find and match the selected chemical name from a given table in the “DATA” sheet with the rows under “MW” column.



Chemical	MW	Volume
NaOH		250
Na2CO3		100
Urea		
Ni(NO3)2		
Co(NO3)2		
Fe(NO3)3		
Mg(NO3)		
Zn(NO3)2		
Al(NO3)3		
CeN3O9.6		
CH3NO3		

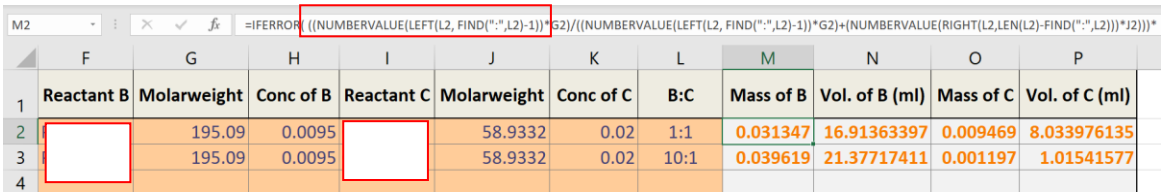
Elements	MW
H	1.00797
He	4.0026
Li	6.941
Be	9.01218
B	10.81
C	12.011
N	14.0067
O	15.9994
F	18.9984
Ne	20.179
Na	22.9898

Figure 3-7: "DATA" sheet

The second sheet was used to implement the formulas in Figures 3-4 and 3-5. In Figure 3-8, the first half of the table was used to calculate the total mass of the other reactant(s) by keying in the fixed mass of the first reactant and total percentage of the other reactant(s).

Name of sample	Reactant A	Fixed mass of A	% of other reactant(s)	Total Mass of other reactant(s)
		2	2	0.040816327
		2	2	0.040816327

Figure 3-8: Table used to calculate the total mass of other reactants



M2 =IFERROR(((NUMBERVALUE(LEFT(L2, FIND(":",L2)-1))*G2)/((NUMBERVALUE(LEFT(L2, FIND(":",L2)-1))*G2)+(NUMBERVALUE(RIGHT(L2,LEN(L2)-FIND(":",L2)))*J2)))*

	F	G	H	I	J	K	L	M	N	O	P
1	Reactant B	Molarweight	Conc of B	Reactant C	Molarweight	Conc of C	B:C	Mass of B	Vol. of B (ml)	Mass of C	Vol. of C (ml)
2		195.09	0.0095		58.9332	0.02	1:1	0.031347	16.91363397	0.009469	8.033976135
3		195.09	0.0095		58.9332	0.02	10:1	0.039619	21.37717411	0.001197	1.01541577
4											

Figure 3-9: Table used to calculate Reactants B and C mass and volume

The figure above shows the second half of the table that was used to automatically calculate either the mass or volume of the other reactants. Elements used for reactants B and C were selected from a list shown in Figure 3-7. Once selected, the MW will be printed out automatically using the method explained earlier. The ratio of the two reactants will then be inputted. Using the “FIND(“:”, L2)” command, the index at which “:” appears in the string can be determined. Therefore, using “LEFT(L2, FIND(":",L2)-1)” as seen in Figure 3-9, the ratio for reactant B can be sliced out as

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

the program reads from the left of the ":". Similarly, using the "RIGHT(L2, LEN(L2)-FIND(":",L2))" command, the program will read from the right of the ":" index to the end of the string. Once both ratios are separated, the formula seen in Figure 3-5 was used to find out the respective volumes and mass for the reactants.

3.4 Catalyst Preparation

3.4.1 Impregnation

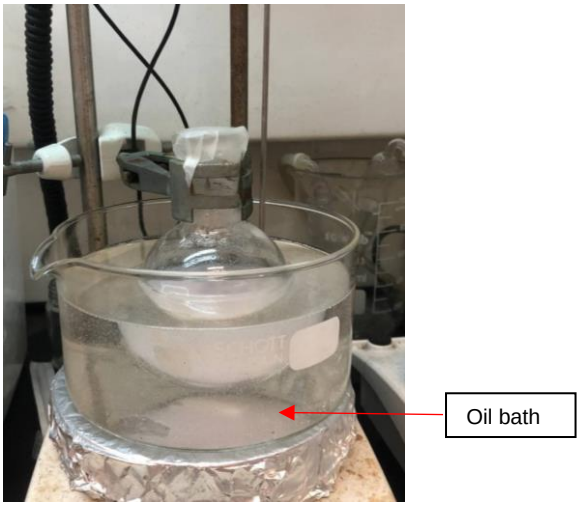


Figure 3-10: Preparation of sample X5

Known as the physical method for catalyst preparation, impregnation is to allow a solid sample to fully absorb a liquid substance. If the solid sample is porous, there will be air bubbles located inside the pores. These act as a void preventing the solid sample to fully absorb the liquid substance. However, rising the pressure and the stirring rate will only reposition the bubbles but are not effective in removing them. Therefore, ultrasound is used to remove such bubbles and allow the solid sample to be saturated with the liquid substance.

3.4.2 Precipitation

Precipitation is a method of obtaining an insoluble solid from two or more aqueous solutions. This preparation method normally occurs at a specific temperature. Optimum conditions such as temperature and pH values are very important to ensure that maximum reaction will occur. If these requirements were not met, the precipitate may not be able to form or only a little amount would be produced.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Figure 3-11: Hot plate and magnetic stirrer

(Home Science Tools, n.d.)

The basic setup includes placing an oil bath onto a hot plate. A magnetic stirrer was used to stir the solution in the round bottom flask (RBF). A retort stand was used to position the RBF into the oil bath. This was to prevent the bottom of the flask from touching the bottom of the oil bath ensuring that the solution in the flask was being heated up evenly. There are two knobs on the hot plate. One is to control the temperature of the plate while the other controls the speed of the magnetic stirrer.

Figure 3-12: Temperature controller

(LabFriend, 2014)

A temperature controller was used to measure the temperature of the oil bath and set it at the reaction desired temperature. Once the desired temperature was reached, the hot plate temperature will no longer increase thus maintaining the oil bath and solution at optimum temperature.

Procedure 1:

Most of the time, the precipitation reaction taking place was a substitution reaction. This reaction occurs when one functional group replaces another functional group. This experiment involved reacting three aqueous clear solutions to form a murky solution containing both solid (precipitate) and aqueous products.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

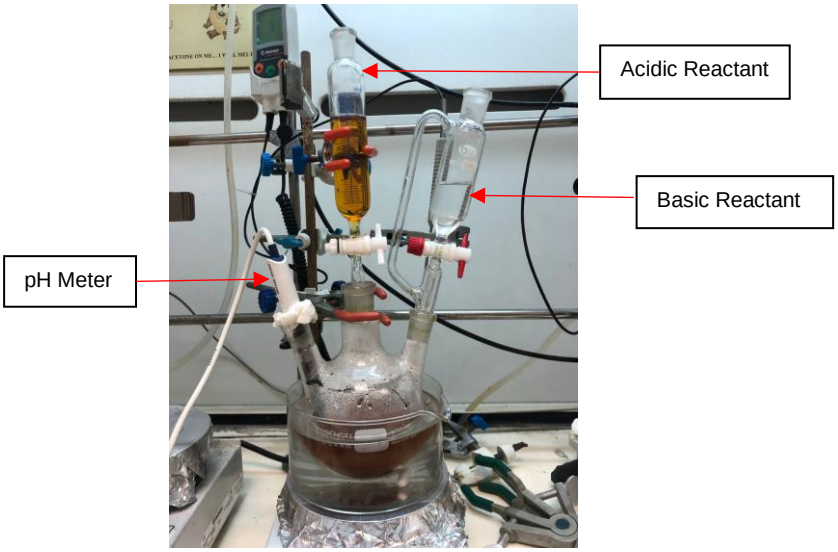


Figure 3-13: Precipitation with 3 reactants

As mentioned earlier, three aqueous reactants were being used for this precipitation preparation. One reactant was poured into the RBF and placed into an oil bath. Whereas the other two reactants, which were acidic and basic solutions, were poured into a burette and added dropwise into the RBF. The flow rate of the acidic reactant was fixed whereas the flow rate of the basic reactant had to be adjusted to ensure the overall solution was at optimum pH. For example, if the pH was too high, the flow rate of the basic reactant must be reduced. Maintaining the solution at a constant pH was difficult as the pH of the solution drastically changes even with 1-2 drops of excess basic or acidic solution. Therefore, this experiment requires a lot of patience and precision.

Figure 3-14: pH meter

(Mettler-Toledo, n.d.)

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

A pH meter was used to measure the pH of the solution in the RBF. This can be seen in Figure 3-13.

Procedure 2:

Figure 3-15: 3ml disposable pipette

(Fisher Scientific, n.d.)

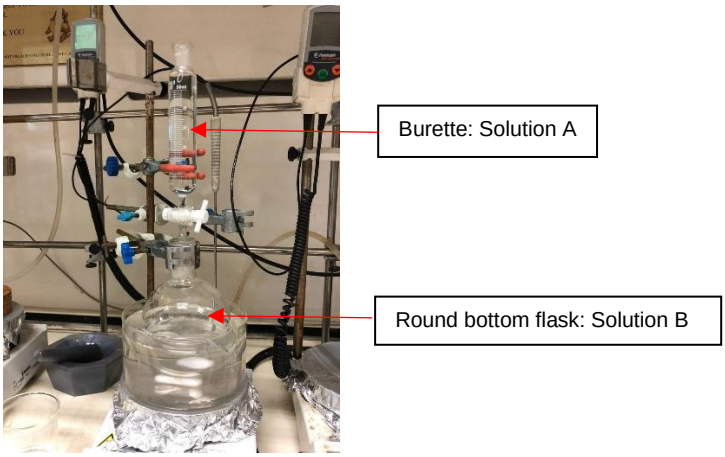


Figure 3-16: Precipitation using a burette

Solution A was added dropwise into solution B using either a burette or a disposable pipette depending on the volume of solution B. As solution A was added to solution B, a precipitate was formed. Once all of solution A was added, the solution is left to age overnight in an oil bath.

3.4.3 Hydrothermal

Hydrothermal is a method of obtaining solid crystals from high-temperature aqueous solutions under high vapour pressure. Crystallisation occurs in the autoclave. During this process, some impurities in the surrounding solution will be rejected by the growing crystal.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

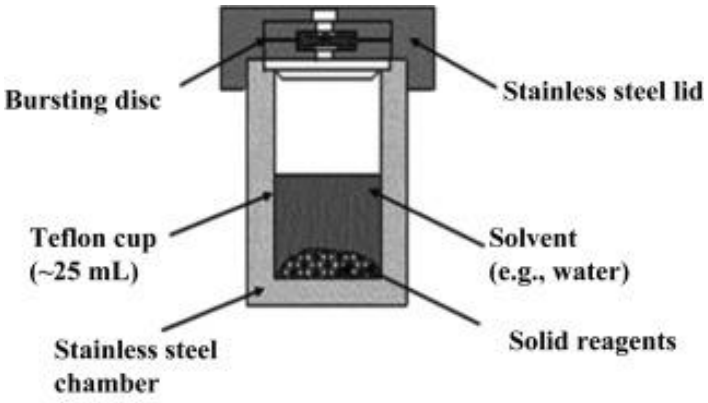


Figure 3-17: Inside an autoclave

(Kaflé, 2019)

Figure 3-18: Breakdown of an autoclave

(Kaflé, 2019)

Procedure

If the sample was a solid sample, it was first grounded using a mortar and pestle and then dissolved in 30ml of DI water. The dissolved sample was then poured into the Teflon chamber of the autoclave (Figure 3-18). If the sample was a liquid solution, it was immediately added into the Teflon chamber of the autoclave.

The chamber will then be capped and placed inside the stainless-steel chamber. A cap and lid were used to close the instrument tightly to ensure no gas can escape. The autoclave was then placed in an oven at optimum temperature for 12hrs to allow the sample to undergo hydrothermal synthesis.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

3.5 Catalyst Collection

The collection method of the catalyst varies based on the amount of sample that was present and its' physical state after preparation.

3.5.1 Filtration

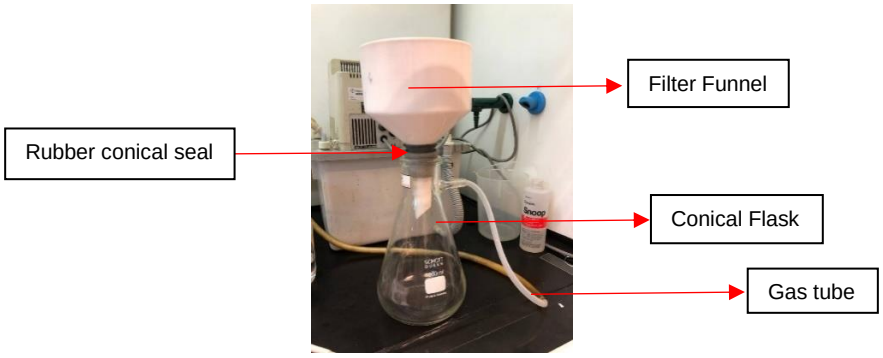


Figure 3-19: Filtration Set-up

Filtration involves the separation of a solute from a solute-solvent solution. The basic filtration setup involves a filter funnel, filter paper and a conical flask. The filter funnel containing filter paper would be placed on the top of the conical flask. The solution containing the sample will be gradually poured into the filter funnel and onto the filter paper. To ensure the flask was hermetically closed, a rubber conical seal was used. The conical flask was attached to a vacuum pump used to draw out air from the flask via a gas tube. Since surrounding air was prevented from entering the flask, the solvent would be suctioned through the filter paper into the conical flask, to occupy the space initially taken up by the removed air. Therefore, the solvent will be separated from the solute. DI water was used to wash the solute 3 times before it was removed along with the filter paper and placed into the oven to dry overnight.

3.5.2 Rotary Evaporation (RE)

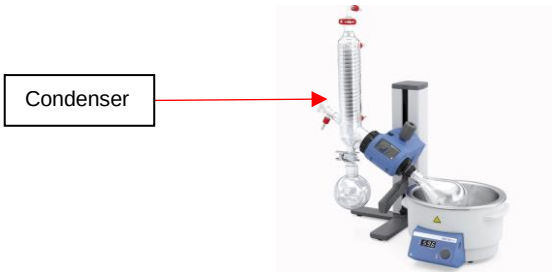


Figure 3-20: Rotatory Evaporator

(Profilab24, n.d.)

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

An RE is used for efficient removal of the solvent, therefore, leaving behind a solid sample. The vacuum pump attached to the RE lowers the pressure in the RBF causing the solvent to have a lower boiling point which in turns promotes evaporation. The rotation helps to increase the effective surface area by forming thin films of the solution on the walls of the RBF. The solvent is removed via evaporation when it is uniformly being heated by a water bath. The evaporated solvent will leave the RBF and into the condenser where it will be converted back to liquid state and fall into a separated RBF attached at the bottom. After all the solvent had evaporated, the solid sample obtained from the solution was placed into the oven to continue to dry overnight.

3.5.3 Centrifuge

Figure 3-21: Conical Centrifuge tube

(Esca Tech Inc, n.d.)

The sample solution was poured into a conical centrifuge tube as shown in Figure 3-21. An additional tube containing DI water (balance tube) was used as a balance to counter the weight of the sample tube. This is necessary for safe operation and prevents damaging the instrument.

Figure 3-22: Centrifuge Rotor

(ProfiLab24.com, n.d.)

Before placing the tubes inside the centrifuge, both tubes had to be weighed to ensure they were of similar weight. Once weighed, the balance tube was placed in the rotor, opposite from the position of the sample tube.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Figure 3-23: Centrifuge
(Arthrex Vet Systems, n.d.)

A centrifuge was used to separate the solid particles from a solution. As the rotor spins the sample tube in the centrifuge, a centrifugal force is being applied onto each particle of the solid sample causing it to sentiment at the bottom of the tube. Therefore, after spinning, the solution was separated into a clear solution and a solid sample which would be suck to the bottom of the tube. The clear solution was then poured out and DI water was added into the tube. A metal spatula was used to scrape the solid sample off the walls of the tube. This was to ensure the sample was thoroughly washed and to get rid of any unreacted solvent. The tube was then weighed again followed by the balance tube which weight will be adjusted accordingly. The tubes were then placed inside the rotor to be span again. This process was repeated 2 more times. After the last spin, the clear solution was poured out and the solid sample left in the tube will be placed in the oven to be dried. If the sample was already reduced, the sample will be placed into a vacuum oven instead to prevent oxidisation in the presence of atmospheric air.

3.5.1 Collecting the dried samples

Figure 3-24: Mortar and pestle
(Laval Lab, n.d.)

After being left in the oven, the sample is taken out. Using a metal spatula, the sample was scraped of either the walls of the centrifuge tube, RBF or the filter paper

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

and into a mortar. A pestle is then used to crush the sample until powder-like. Refer to Appendix B1 for the calcination of the catalyst.

3.6 Challenges Faced and Learning Points

During the split teams, I was faced with many challenges. Firstly, I was given a list of tasks to complete before the end of the week. In hopes to meet the deadline, I had to maximise my productivity. This meant that I had to conduct more than one experiment at once. At first, this was stressful but after much practice, I was able to get a hang of it. Planning out my time became an essential skill for me to finish my task for the week. An example would be while preparing two catalysts back-to-back, it was important to decide when to start preparing the second catalyst. This was so that when the first catalyst was done ageing, I can place the second batch into the oil bath without having to wait for it to heat up. Since both the DRIFTS experiment and preparation of catalyst had a long waiting time in between, I was also able to learn the art of multi-tasking. While conducting the DRIFTS experiment, on one hand, I was preparing various catalysts on the other. This saved a lot of time and helped me finish my task before the end of the week.

Secondly, I had to learn how to be independent and to be adaptable to my surrounding. I was faced with many obstacles such as a spoiled fume hood and was only limited to two power outlets. Therefore, during the preparation of the catalyst, I had to plan which two instruments I should turn on first followed by the other. Without the help of Xiao Xin there, troubleshooting was also something I had to learn to do independently. Using new instruments led me to make some mistakes. For example, I had some difficulty with using the high-speed centrifuge. After testing out various measures, I realised that there was a limit on the weight of the centrifuge tube loaded into the rotor. With more practice, I learned the ability to think on my toes and to make the most out of the resources I had.

Personal responsibility can be practised in many areas. Honestly and owning up to your mistakes contributed to one of these areas. Most of the time, I naturally felt very ashamed for making a mistake. Since the experimental results can be easily altered by a preparation mistake, it was important for me to make these mistakes known. For example, I once accidentally spilt the solid reactant onto the fume hood when

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

adding it into the RBF. Knowing that the performance of the catalyst will be affected, I chose to tell Xiao Xin. It was embarrassing at first, but I knew that if I were to keep them to myself, it would have led to more severe consequences. Mistakes are bound to happen, but one should always take responsibility and learn from them. After that incident, I learnt to be more careful when adding the solid reactant into the RBF. Sometimes, I would place a weighing paper below to catch any spillage.

Another area I practised personal responsibility is by taking pride in my work. The presence of contamination in the catalyst prepared will jeopardise the reliability and accuracy of the experimental results. From dirty stirring bars to the falling of dirt into the sample, there are many ways for the sample to be contaminated. The best way to avoid this was to take extra precautions. Washing the instruments thoroughly before they were used was just as important as the preparation itself. In school, during practical lessons, we are taught that taking shortcuts can lead to facing complications in the future. For example, by not conducting a faulty test on the components, a faulty component may be soldered onto the printed circuit board causing the whole circuit to not work. Similarly, when preparing the catalyst, laziness cannot be tolerated, and every step had to be followed with the utmost attention and focus. Therefore, in everything that I do, I had to ensure that I was giving my best to produce quality work or experimental results.

I was able to program an Excel sheet containing various calculation tables to help minimise calculation errors. It was difficult to find the exact code I needed for each cell to execute the desired task. However, after doing some research and referencing from sample codes, I was able to get a basic understanding of the commands needed and how their functions interplay with each other. To better improve the aesthetic, I was able to implement “IFERROR()” or “IF()” statement to leave the cell empty until a valid value had been calculated. The excel sheet also allowed me to log in all my previous calculations to refer to in the future. I was able to test my creativity when designing the layout and flow of the table. This was a great opportunity for me to value add to the project using an expertise that I was more familiar with.

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Chapter 4. Python

4.1 New Concepts

Using self-paced packages, various new concepts on the programming language, python, were taught and practised on the software, Jupyter Notebook.

4.1.1 Arrays

```
a = "Hello, HippoPotamus!"
print(a[3]) #print the 4th letter
#space inclusive
print(a[: -4]) #1st to 16th character
print(a[1:-2]) #2nd to 18th character
print(a[2:5]) #3rd to 5th character
print(a[-5:-2]) #15th to 18th character
print(len(a)) #Length of string
print(a.strip())
print(a.lower())
print(a.upper())
print(a.replace("H", "J"))
print(a.split(","))
x = "ppo" in a #Check if the phrase "ppo" is present
print(x)
x = "mus" not in a
print(x)
```

```
l
Hello, HippoPota
ello, HippoPotamu
llo
amu
20
Hello, HippoPotamus!
hello, hippopotamus!
HELLO, HIPPOPOTAMUS!
Jello, JippoPotamus!
['Hello', ' HippoPotamus!']
True
False
```

Figure 4-1: Strings in python

In Python, strings are treated as arrays. Therefore, each character including spacing has a respective index. The sections or characters of a string can be sliced or replaced. If a string has multiple words, the command ".split()" was used to separate these words. Another unique command used with strings is the "in" or "not in" command. This command checks for the presence of one string in another. The output of this command was either true or false. The index count starts from 0. To count from the back of the string, negative indexes are used as seen in Figure 4-1. The command "<arrayname>[start:end]" allows slicing of the string by stating the starting and ending indexes of the slice. The character represented by the ending index will not be included in the slice.

Later in the package, NumPy was introduced. This is a python library used for working with arrays. An additional feature was implemented when slicing a NumPy array using the "<arrayname>[start:end:step]" command. The variable "step"

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represents the index increment of the slice produced. This can be done on standard python strings as well. As seen in Figure 4-2, this command can be used to reverse the order of an array

```
#part 3
b = np.arange(10,20)
b = b[::-1]
print(b)
```

```
[19 18 17 16 15 14 13 12 11 10]
```

Figure 4-2: Reverse the order of array

By setting the step to -1, the array was printed from the last index to the first. Another way to reverse this order was by using the command “np.flip(<arrayname>, x)”. As shown in the figure below, the variable “x” can either be set as 0, 1 or None depending on the array’s dimension and the order in which the user wants to reverse the array.

```
#part 4
c = np.arange(9).reshape(3,3)
#reverse rows
d = np.flip(c,0)
print(d)

#reverse numbers in each row
e = np.flip(c,1)
print(e)

#reverse number and rows
f = np.flip(c)
print(f)
```

```
[[6 7 8]
 [3 4 5]
 [0 1 2]]
[[2 1 0]
 [5 4 3]
 [8 7 6]]
[[8 7 6]
 [5 4 3]
 [2 1 0]]
```

Figure 4-3: Numpy array and “.flip()” command

One unique feature that differentiates a NumPy array from the standard python array is the use of dimensions, also known as axes. A multidimensional array is a table consisting of elements of the same data type. Each element is indexed by a tuple of non-negative numbers. The command “np.arrange(c,d)” will generate a flat integer array with numbers starting from “c” to “d”. The NumPy array created in the figure above contains integers starting from 0 to 9. To add dimensions to this flat array, the command “.reshape()” was used. As shown in Figure 4-3, If x = 0, the order of the

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rows along the x-axis will be reversed. If x = 1, the order of numbers in each row along the Y-axis will be reversed. Lastly, if x = None, both the number and rows of the arrays will be flipped.

```
#exercise 18
import numpy as np
myarray = np.array([ [1, 2, 3, 4, 5], [6, 7, 8, 9, 10], ['a', 'b', 'c', 'd', 'e'] ])

print(myarray[2, 1:4]) #Try 0 to 2

print(myarray.shape)
```

```
['b' 'c' 'd']
(3, 5)
```

Figure 4-4: Slicing NumPy array

The NumPy array created in the figure above has the dimension of (3,5) indicating that it has 3 dimensions, and each dimension has 5 elements. The command ".shape()" will output the dimension of the NumPy array. To slice a multidimensional array, the desired dimension is selected by stating the dimension followed by a "," and then the desired slice is determined by stating the start and end indexes.

```
In [32]: import numpy as np
         #part 1
         a = np.zeros(10) #array/vector of zeros
         print(a)

         d = np.random.random((3,3))
         print(d)
```

```
[0. 0. 0. 0. 0. 0. 0. 0. 0. 0.]
[[0.62734421 0.37768667 0.07539265]
 [0.50865377 0.45790178 0.73262842]
 [0.61332062 0.01090004 0.67614084]]
```

```
In [3]: #part 2
        a = np.ones(10) #array/vector of ones
        print(a)
```

```
[1. 1. 1. 1. 1. 1. 1. 1. 1. 1.]
```

Figure 4-5: Alternate ways to generate NumPy arrays

There are various ways of generating a NumPy array. For example, "np.zero(num)" or "np.ones(num)" used in Figure 4-5 will produce an array with the stated number of zeros or ones, respectively. The random library in python can also be implemented to produce a multidimensional NumPy array containing randomly generated elements. This was done by using the command "np.random.random" followed by the desired dimension of the array as seen in Figure 4-5.

4.1.2 Data structures

In python, there are four built-in data structures. Firstly, a list is a data structure that makes use of a single variable to store multiple items. "[ ]" brackets are used to enclose these items. There are different commands used to execute different tasks.

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As mentioned before, indexes are used to differentiate the different items in the list starting with 0.

```
#exercise 9

n_list = [1, 2, 3, 4, 5]

# adding element 100 at the fourth location
n_list.insert(3, 100)
print(n_list)

# adding element at the end of the list
n_list.append(99)
print(n_list)

n_list.extend([11, 22, 33])
print(n_list)

n_list.clear()
print(n_list)s
```

```
[1, 2, 3, 100, 4, 5]
[1, 2, 3, 100, 4, 5, 99]
[1, 2, 3, 100, 4, 5, 99, 11, 22, 33]
[]
```

Figure 4-6: Commands used for List

The command ".insert()", ".extend()", and ".append()" commands are used to insert item(s) into the list. As seen in the figure above, ".insert()" will add in an item at a given position. Whereas, ".extend()" will add multiple items and ".append()" will add one item to the back of the list. There are plenty of other commands that can be used to make changes to a list. For example, the command ".remove()" get rids of the desired element in a list and the command ".clear()" can be used to empty out the entire list.

```
#exercise 11
list1 = ["a", "b" , "c"]
list2 = [1, 2, 3]
list3 = list1 + list2
print(list3)

for x in list2: #alternative way
    list1.append(x)
print(list1)
```

```
['a', 'b', 'c', 1, 2, 3]
['a', 'b', 'c', 1, 2, 3]
```

Figure 4-7: Addition of List

There are also ways of combining two lists. Firstly, one can do this by adding both lists together using a "+" operator. Another way is to use a for loop to individually add the items in one list to another as seen in the figure above.

```
---------------------------------------------------------------
---------------
TypeError                                 Traceback (most re
cent call last)
<ipython-input-3-18c9171b681d> in <module>
      1 print(Fruittuple[2:5])
      2
----> 3 Fruittuple[3] = "orange" # This will raise an error

TypeError: 'tuple' object does not support item assignment
```

Figure 4-8: Error Message

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Besides lists, tuple is another built-in data structure that holds multiple items in one variable. Unlike lists, these items cannot be changed as they are fixed to the order that they were declared as. The error message shown in Figure 4-8 will appear if the user attempts to alter a tuple. To add any changes to a tuple, users can convert it to a list and then back to a tuple after making their changes.

```
#exercise 15
names = ("John", "Peter", "Liza", "Linda", "Zasp")
(white, yellow, *black) = names
print(white)
print(yellow)
print(black)
```

```
John
Peter
['Liza', 'Linda', 'Zasp']
```

Figure 4-9: Splitting up a tuple

To identify a tuple, "()" brackets are used to enclose the items in a tuple. In Figure 4-9, the items in a tuple can be split up and assigned to multiple variables. When the symbol "*" is added before a variable name, the rest of the items in the tuple not stored in other variables will be store in this single variable.

```
: #exercise 20 : set
myset = {"apple", "banana", "cherry"}
myset.add("orange")
print(myset)

myset.update(["apple", "mango", "grapes"]) # Add multiple items to a set
print(myset)

set1 = {"a", "b" , "c"}
set2 = {1, 2, 3}
set3 = set1.union(set2)
print(set3)
```

```
{'orange', 'apple', 'cherry', 'banana'}
{'banana', 'grapes', 'orange', 'apple', 'cherry', 'mango'}
{'a', 1, 2, 3, 'c', 'b'}
```

Figure 4-10: Various commands used for sets

The next data structures are sets that are also used to store many items in one variable. These items are enclosed by "{ }" brackets. To add one item to the set, the ".add()" command can be used. However, to add multiple items, they are typed out as a list and the ".update()" command can be implemented instead. When ".update()" command is used, it is important to note that duplicates will not be added to the set as seen in Figure 4-10. Multiple sets can be added together to form a bigger set by using the ".union()" command. The order of the items in the new set depends on which set is called first.

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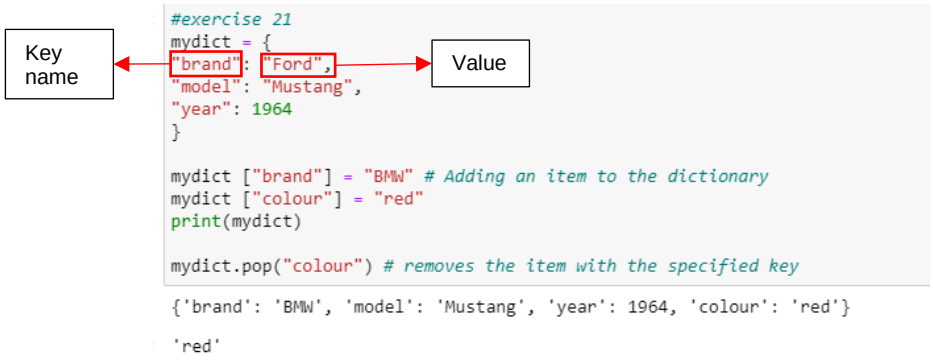

Figure 4-11: Dictionaries

The last data structure is dictionaries which is an ordered collection of key: value pairs. Duplicates are not allowed in such dictionaries, but the contents in dictionaries can be changed. In Figure 4-11, the statement "<dictionaryname> [<keyname>] = "<newitem>" is used to add or replace items in a dictionary. Using the ".pop(<keyname>)" can be used to print the value stored under the desired key. The values stored under the various keys can also consist of other data structures as shown in Figure 4-12.

4.1.3 JavaScript Object Notation (JSON)

JavaScript Object Notation (JSON) is a syntax that can be used to store and transfer data. This syntax is normally used for web applications. Serialisation is the process whereby the JSON text is encoded into a series of bytes to be transmitted over the network. This process is needed to write or read a data file.

Figure 4-12: Using JSON to write into data files

To code using the JSON, the python JSON library must be called with the "import json" command. In Figure 4-12, the variable "x" which is a dictionary consisting of various other data structures is written into "data_file.json" file. Firstly, the data file "data_file.json" is opened in the writing mode using "w". A new JSON file will be

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created under the given name if it doesn't exist. Once opened, the command "json.dump()" converts the variable "x" into a JSON string which is stored in "data_file.json".

```
with open("data_file.json", "r") as read_file:
    data = json.load(read_file)
data['hobbies']
```

```
['eating', 'sleeping', 'shitting']
```

```
data['children'][0]['age']
```

```
6
```

```
for i in range(0,len(data['children'])):
    print(data['children'][i])
```

```
{'firstName': 'Ah Beng', 'age': 6}
{'firstName': 'Ah Lian', 'age': 8}
```

Figure 4-13: Using JSON to read data files

Figure 4-13 uses "open()" function to read the JSON file, "data_file.json" by changing the "w" to "r". The contents in the file are parsed using the command "json.load()" and stored in the "data" variable as a dictionary. Dictionaries, lists, and sets were used to differentiate the information stored in "data" allowing the user to display or print certain sections of the entire data file. Data files can be excess in any notebook and at any time.

4.1.4 "datetime64" datatype

The "datetime64" datatype involves the use of different date, time units and the abbreviation, 'D', used in the figure below stands for days. Using a NumPy array ".arrange", the start and end values are set to the desire dates using the format "YYYY-MM-DD" which are valid NumPy date objects. The datatype of the NumPy array must be set to 'datetime64'.

```
#part 1
import numpy as np
print("July, 2021")
print(np.arange('2021-07', '2021-08', dtype='datetime64[D]'))

print(np.arange('2021-07', '2021-08', 2, dtype='datetime64[D]'))
```

```
July, 2021
['2021-07-01' '2021-07-02' '2021-07-03' '2021-07-04' '2021-07-05'
 '2021-07-06' '2021-07-07' '2021-07-08' '2021-07-09' '2021-07-10'
 '2021-07-11' '2021-07-12' '2021-07-13' '2021-07-14' '2021-07-15'
 '2021-07-16' '2021-07-17' '2021-07-18' '2021-07-19' '2021-07-20'
 '2021-07-21' '2021-07-22' '2021-07-23' '2021-07-24' '2021-07-25'
 '2021-07-26' '2021-07-27' '2021-07-28' '2021-07-29' '2021-07-30'
 '2021-07-31']
['2021-07-01' '2021-07-03' '2021-07-05' '2021-07-07' '2021-07-09'
 '2021-07-11' '2021-07-13' '2021-07-15' '2021-07-17' '2021-07-19'
 '2021-07-21' '2021-07-23' '2021-07-25' '2021-07-27' '2021-07-29'
 '2021-07-31']
```

Figure 4-14: Printing out the days in July 2021

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

In Figure 4-14, a NumPy array containing all the corresponding dates of the days in July 2021 was generated. By adding the step feature into this statement, the desired number of days will be skipped while the rest is stored inside the NumPy array. For example, If the step was set to 2 as shown in the figure above, only the dates of the odd days in July 2021 were printed out.

```
print(np.arange('2021-07', '2022-07', dtype='datetime64[M]'))
```

```
['2021-07' '2021-08' '2021-09' '2021-10' '2021-11' '2021-12' '2022-01'
 '2022-02' '2022-03' '2022-04' '2022-05' '2022-06']
```

Figure 4-15: Printing out the month from July 2021 to 2022

If the abbreviation was changed to this to 'M', the array printed out will only show the months between the start and end dates provided as seen in Figure 4-15.

4.2 Random Number Guessing Game

This project makes use of the random library in python to generate a random number within a given range. Once the number has been generated the player is tasked to guess this number. The player will have 8 tries to guess the number correctly.

```
Enter your guess:90
Too low! try again
Enter your guess:95
Too high! try again
```

Figure 4-16: Hints are given to the player

After each incorrect guess, the game will provide a hint about whether the player's previous guess was too high or low. If the player guesses the number correctly, one point is added to their score and the player will advance to the next level as seen below. Each time they advance, 100 more possible numbers will be added to increase the difficulty. The number of tries will return to 8 tries at the start of each level. The game will end only when all 8 tries are used.

```
Enter your guess:91
Correct! Your score is 1
Start playing LEVEL 2
Enter your guess:201
Invalid input!! Please keep within the range
Enter your guess:\
Invalid input! Please input an integer!
Enter your guess:9.4
Invalid input! Please input an integer!
```

Figure 4-17: Error messages

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

The program also checks if the player's input is valid. Using the command ".isnumeric()", the program will be able to prevent the player from entering special characters or letters. If-else statements were then used to ensure the number keyed in by the player is within the given range. If the player's input does not meet all the requirements, an "Invalid" message will be printed. An invalid input will not contribute to the try count.

```
Start playing LEVEL 1
Enter your guess:9
Too low! try again
Enter your guess:0
Too low! try again
Enter your guess:0
Too low! try again
Enter your guess:0
Too low! try again
Enter your guess:0
Too low! try again
Enter your guess:0
Too low! try again
Enter your guess:0
Too low! try again
Enter your guess:0
Too low! try again
Enter your guess:0
Too low! try again
Game Over! Your score is 0
Do wish to play again?(Y/N)n
```

Figure 4-18: User interface if the player chose not to continue playing

```
Too low! try again
Enter your guess:8
Too low! try again
Game Over! Your score is 1
Do wish to play again?(Y/N)y
Start playing LEVEL 1

Enter your guess:
```

Figure 4-19: User interface if the player chose to continue playing

Once the player has run out of tries, the game will end, and the player's final score is displayed. The player will then be prompted if they wish to play again or to stop playing. As seen in Figure 4-19, if the player chooses to play again the level restarts back to 1. The score will also reset back to 0. Refer to Appendix C1 to view code.

4.2.1 Challenges and Improvements

Firstly, the variable used to control a for loop cannot be altered using commands inside or outside the loop. This variable was solely used to control the loop alone and can only be altered when the for loop was introduced. Therefore, a while loop was used instead to control the number of tries the player had. This is so that the variable "i" can be altered by commands from other parts of the code.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

```
if (user.is_integer()):
    user = int(user)
```

Figure 4-20: ".is_interger()" command

As seen in the figure above, the command ".is_integer()" was used originally. This command will return a true only if every character of the player's input was an integer. However, when the player inputs special characters, letters or floats, the software will show an Error message. To tackle this problem, more research was done and this command was changed to ".isnumeric()".

```
Start playing LEVEL 1?(Y/N)Y
32
Enter your guess:3
Too low! try again
Enter your guess:32
Correct! Your score is 1
Start playing LEVEL 2?(Y/N)Y
Enter your guess:exit
Invalid input! Please input an integer!
Enter your guess:-
Invalid input! Please input an integer!
Enter your guess:32
Correct! Your score is 2
Start playing LEVEL 3?(Y/N)32
Enter your guess:4
Too low! try again
Enter your guess:4
Too low! try again
Game Over! Your score is 2
Do wish to play again?(Y/N)N
```

Figure 4-21: Error with game

Originally, when the function "randnum()" was created, there was some issue with generating a new number for each level. After some troubleshooting, it was discovered that the variable "num" was not declared as a global variable. Hence, its' value cannot be changed by commands outside of the function it was declared in.

```
while x.upper() == 'Y':
    num = random.randrange(y)
    while i<8:
```

Figure 4-22: Initial code

Before changing to calling the "randnum()" function, the statement above was initially used to generate the random number for level 1. However, when the function "randnum()" was later called in the code, the program treated the variable "num" in Figure 4-22 as a separate variable from the "num" used in the function. Therefore, function "randnum()" was not able to alter the "num" variable used in the code above. This led to the correct number for each level to be the same as in Figure 4-21.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

This mistake was also observed with the variable “i”. If not for declaring “i” as a global variable, the player will have endless numbers of tries. Since “i” cannot be altered by the “i = i + 1” command used outside of the function, the value of “i” remains at 0. Therefore, when adding in functions, it was important to make sure variables used in multiple functions were declared as global variables.

4.3 Fast-Food Restaurant Ordering System

The Fast-Food Restaurant Ordering System helps to take the customers’ orders and calculate their total bills. The food options include burgers, sides, and drinks and each option has three different choices. This is shown below.

```
======= MENU =======
Burgers($10): ['Chicken Burger' 'Beef Burger' 'Fish Burger']
Sides($5):    ['Fries' 'Nuggets' 'Salad']
Drinks($2):   ['Coke' 'Sprite' 'Fantagrape']


Meal option(includes burger, sides and drink): $15
Students Discount(Weekdays): 50%
==================

How to order?
KEY IN 0/1/2/3 for each the food
0:None of the choices
1:First choice
2:Second Choice
3:Third Choice
Example:
Enter your burger order: 1
Enter your side order: 0
Enter your drink order: 3
= Customer ordered a Chicken Burger with NO sides and a Fantagrape
```

Figure 4-23: Fast Food Restaurant menu

The customer will then be prompted separately to choose either 1,2,3 or none of the choices for each food option. If they have ordered all 3 food options, the program will then provide them with a cheaper option of converting their order to a meal as seen below.

```
Enter your burger order:1
Chicken Burger
Enter your sides order:0
Chicken Burger
No sides
Enter your drinks order:2
Chicken Burger
No sides
Sprite
Would you like to confirm you order?(Y/N):n
Order More Food?(Y/N):y
Enter your burger order:3
Fish Burger
Enter your sides order:2
Fish Burger
Nuggets
Enter your drinks order:4
Please stay within the range(within 0 to 3)!!
Enter your drinks order:n
Invalid Input!!
Enter your drinks order:1
Fish Burger
Nuggets
Coke
Would you like to confirm you order?(Y/N):y
Do you want a meal?(Y/N):y
Order More Food?(Y/N):n
```

Figure 4-24: Example Order

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

After each prompt, the program will print the customer's most recent order. The program will also check if the customer's input meets all the requirements. Special characters and letters will trigger an "Invalid Input" message. Numbers exceeding the range of 0 to 3 are also not acceptable. The customer will continue to be prompted again for the same food option until they key in a valid number. Once the customer has key-in valid inputs for all three food options, they will be asked if they would like to confirm their order. If the customer inputs 'y', the order will be recorded down. If not, it will be deleted. Next, the customer will be prompted if they wished to order more food. The customer can key in as many orders as they wish.

Figure 4-25: Example display of final bill

As seen in the figure above, a bill will be printed upon completing the orders. The bill will display the cost of each order as well as the customer's food choices. The total cost before and after GST and service charge will be calculated and displayed.

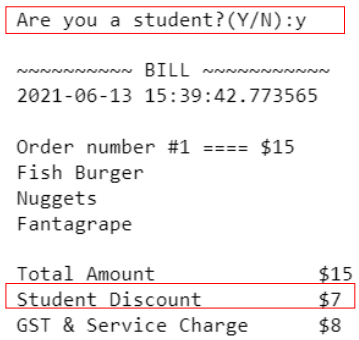

Figure 4-26: Student Discount

A 50% student discount is also available but only on weekdays. Upon completing their order, the customer will then be asked if they are a student. if they reply with a 'y', half of the customer's bill will be deducted before the GST and service charge is added. Refer to Appendix C2 to view code.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

4.3.1 Challenges and Improvements

```
How to order?
KEY IN 0/1/2/None for each the food separated by a spacing
Example: "0 None 2" = Chicken Burger and Fatagrape
```

Figure 4-27: Initial instructions for ordering

One aspect that needed a lot of improvement was the user interface. Initially, the user was supposed to key in either 0, 1, 2 or None to select their desired food choice. To ease ordering and validating the customer's order, this was switched 0 to 3, 0 being not wanting any food and 1 to 3 representing the food choices, respectively. To make ordering more convenient and easier to understand, the ordering system was also changed to ordering the food choices individually instead of together. Printing out the most recent order showed the program's interaction to the customer's input. This allowed the customer to be able to double-check their order before confirming it.

Another difficulty was deciding how to store the order and cost values. A NumPy array was initially created using the command "np.arrange(15)". However, after doing some testing, the values of each index were fixed and cannot be altered. After more research, it was decided to use an empty list. The command ".append()" allows the most recent orders and cost to be store into the list. The use of global variables "odr" and "c" made storing the cost and order more ideal as the values could be easily altered and only added to the list when the customer has confirmed their order.

```
UnboundLocalError                         Traceback (most recent call last)
<ipython-input-6-e5d6a4100c60> in <module>
     69     c = 0
     70     #order meal
---> 71     b = numeric('burger', 0, bc)
     72     s = numeric('sides', 1, sc)
     73     d = numeric('drinks', 2, dc)

<ipython-input-6-e5d6a4100c60> in numeric(name, index, price)
     51                     else:
     52                         odr = odr + '\n' + store(index,user)
---> 53                     c = c + price
     54                 else:
     55                     odr = odr + '\nNo ' + name

UnboundLocalError: local variable 'c' referenced before assignment
```

Figure 4-28: Error Message for the wrong declaration

Another lesson learnt is that global variables must be declared the first time it was introduced in the code. This applies even if they are found in the function that was called later on. If they were not declared, the program will treat the variables as local variables and will not recognise them outside the function. An Error message will be printed out as seen in the figure above.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

4.4 Overall Challenges and Learning points

Throughout the progress of programming the two projects, I was able to test my understanding of what I have learnt in the python packages and challenge myself to program from scratch. It allowed me to explore the various possibilities when using python to code. As I faced many difficulties, I was able to learn useful tips when programming in which I hope to apply in future projects.

Firstly, I was able to learn the importance of planning out my code before actually programming it. This helped me better visualise the flow of the program and write down the various functions that I wanted to include. With so many features to add to the program, it was important to decide and organise which feature comes before the others. As learnt in school, the use of comments sets as important reminders of what each section of the code was programmed for. This help with troubleshooting as it eased finding the section of code that was responsible for causing the error. Print statements were also used for troubleshooting. It helped to narrow down the root cause of the problems encountered. For example, when facing the error when the player was given an infinite number of tries, I use print statements to print the value of the integer “i” and was able to realise that the integer had to be set as a global variable.

Another lesson I learnt was that the User’s interface plays a big part in the project. Since I am programming projects that require a user’s interaction, the user interface should be kept easy to use and understand. Taking references from similar projects helped me discover what I can add to improve my user’s interface. Small features, such as printing out the user’s order after they input their choices, is a good way of providing the necessary responses to each input.

Lastly, one very important skill that I learnt was to use my creativity to improve my programs. Many additional features can be added to a simple program to make it more complex and unique. The thirst to improve plays a huge part in my learning especially since there are many accessible reference codes and projects online. With the help of such reference, the possibilities of what I can implement to better my program are endless. An example would be changing the “.is_interger()” to “.isnumeric()” to prevent special characters and letters to be inputted by the user.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Another example is adding the ".upper()" to convert the user's input to upper case. Although this is a very small improvement, it can help ease the user's experience when using my program. I hope to continue to explore my knowledge of python and test my understanding by programming more projects in the future.

Chapter 5. Reflection and Conclusion

5.1 My accomplishment

Over the course of the 22 weeks in ICES, I am happy to see myself learn both hard and soft skills. Before my internship, I was rather nervous as I knew that I would be lacking in my chemistry knowledge but also excited to learn new things. Motivated by the goals I set out for myself, I was able to step out of my comfort zone and ask questions as well as contribute my opinion to improve the project.

I think my biggest accomplishment was to contribute to the DRIFTS project given that I started off with little knowledge about DRIFTS. Through reading and researching more about the science and concepts behind the project, I gained a better understanding of what I was doing. With this newfound knowledge, I could better brainstorm different ideas on how to improve our experimental results. Given the opportunity to do hands-on work under the direct coaching of my lab partner, Xiao Xin, I was able to adapt to my assigned task more effectively. Through practice, I became more familiar with analyzing and inferring from the plotted spectra. Pointing out and evaluating the various details and changes in the spectra has allowed me to better conceptualize ideas to improve the experiment. I also learnt to communicate and listen objectively to the ideas and suggestions from Dr. Liu Yan and Xiao Xin. This has helped expose me to the way they think and to their endless number of ideas and innovations. As I juggle different assigned tasks, I have learnt the importance of efficiency and time management. Conducting experiments independently has given me a sense of responsibility and satisfaction especially when we obtained our desired results.

Due to the new covid restrictions, Xiao Xin and I will be working in split teams. Initially, it was very stressful and scary to be working alone. Xiao Xin will pass me a list of the different experiments he needs me to complete by the end of the week.

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The list normally consists of 5 different experiments or tasks. At first, I was afraid that I would not be able to complete all the tasks by the end of the week. However, after writing out them down and planning my time out, I was able to finish all my assigned tasks on time. Working with a deadline was quite stressful as I had to conduct multiple experiments and preparations at the same time. By taking things step by step, I was able to stay calm throughout the experiment. I did encounter some difficulties when conducting new experiments or preparing new samples. Since the instructions were typed out for me, it was very hard to visualise the experiment and how I was supposed to carry it out. However, recapping back to my observation when Xiao Xin conducted similar experiments, I was able to grasp a rough idea of how to carry it out. I am very happy to be able to transition from conducting only DRIFT experiments with Xiao Xin help to preparing catalysts and finally doing both experiments at the same time independently.

As I worked from home, I am very grateful to be able to learn python and program two projects. With programming knowledge from school, I was able to pick up the various basic python codes and adjust to the new language easily. Programming the project was also a huge accomplishment as I was able to learn new python features and test my understanding. Being able to code using python is an important skill as the language itself is widely used for many applications.

Being able to value add and contribute to the project was a huge achievement for me. Although I had a lack of experience in this field, I was still able to provide small useful inputs here and there. For the DRIFTS experiment, I was able to bring about the change in the spectra unit to Absorbance so that lower energy level catalyst could be tested using DRIFTS. Creating templates also help to speed up the completion of the workload. I was also able to apply my knowledge in programming to help with the calculations done before the preparations of the solutions and catalysts. This was done in hopes to reduce calculation errors and ease calculations.

Overall, I would say that I have gained a lot from my internship at A*STAR. I am beyond lucky to be able to contribute to a research project and deepen my understanding of what it takes to be a researcher.

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5.2 Mentorship

For the past 22 weeks of my internship, my supervisor Dr. Liu Yan served in the role as my mentor and boss. Every 2 weeks, we would meet to discuss the project progress and the next steps to be taken. This made me feel welcome as part of the team and to observe how the team worked. During this meeting, she would always mention the different ways I could help with the project and made sure that I understood what I was doing. Her constant encouragement really boosts my confidence to ask questions to clear any of my queries. I was also given the opportunity to contribute my thoughts and ideas during such meetings. She assigned Xiao Xin as my student buddy and to guide me in the lab. I am very thankful to be able to work under such a caring and understanding supervisor who is willing to help her interns succeed in their internship program.

I thoroughly enjoyed working with my student buddy Xiao Xin. Throughout the internship, he was always very helpful and showed a lot of interest in answering my questions. He always made a point to check if I was coping well with the task assigned. I appreciate his willingness to teach me new concepts. His constant encouragement and confidence in me motivated me to continue giving my best as I hope to show my gratitude by excelling in my work.

5.3 Self-reflection

Being at A*STAR has taught me many valuable lessons. In any scenario, be it to lend a helping hand or to ask questions, taking initiative was an important skill to have. With a lack of experience, I always thought that I would not be of much help. I soon realised that this was false. As long as I am willing to help, I will be able to contribute. All the times I had finished my task early, I would always ask Xiao Xin if there was more to do. By stepping out of my comfort zone, I was able to gain more exposure and learn many new things. I believed that taking initiative could also interplay with taking charge of my learning. Asking questions and sharing my ideas during meetings was quite nerve-wracking at first. However, I realised that I should not be afraid of saying the wrong thing or providing “useless” inputs. I was here to learn, and I knew that no one will be able to help me if I did not bother asking. Expanding my knowledge by reading various references encouraged me to

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contribute more of my suggestions as I was better equipped to give them. I truly believe an intern can add value to the organization by taking the initiative to learn and doing a good job on what she has been assigned.

Although the research I am doing may not relate to biomedical engineering, I could still apply various skills that I learnt in school to my work. For example, taking the utmost responsibility to carry out my task in the best way possible. In school, our grades are normally jeopardised by the quality of the work we hand in. Similarly, our experimental results will be poorly affected at work if we did not follow the instructions carefully and did not take pride in each experiment. To uphold the company's good reputation, I ensure that I gave my best in every task and work assigned to me.

As I worked with my lab partner, Xiao Xin, I was able to understand the importance of teamwork. Although I was just an intern, Xiao Xin was always very supportive of my ideas and inputs to the experiment. This made me realised the importance of being open-minded to others' opinions and having mutual respect for my teammates. Teamwork was something that I also picked up in school. Through group projects, I learnt the importance of effective communication with my teammates. At work, I was able to observe effective communication between the other scientists and Xiao Xin. During discussions, all the teams' views and ideas were being listened to and taken into consideration when finding new ways to improve the project. I was also able to practice teamwork as most of the tasks done in the lab and plotting the experiment data were divided between Xiao Xin and I. When faced with problems, Xiao Xin and I would always brainstorm together to find the best way to tackle the problem. Teamwork is an essential skill to have as I am bound to meet and work with others in both, school, and work, in the future.

When experimenting, one encounters more failures than success. However, it was important to always learn from such failures and to always look for new ways to improve. Through reading and referring to reference literature, we not only learn from our failures but also that of others. As there is no guaranteed outcome, these failures may lead to new discoveries. Therefore, no failure is deemed as a waste. In programming, we are taught that the learning never stop as there are endless possibilities that one can program. Research is like that as well. There are many

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approaches to tackling a problem, but the important thing was finding the best one even if that meant trying everything. Through this, I learnt to never be afraid to try and make mistakes as there is still so much for me to learn.

As mentioned earlier, meeting failures was a very common encounter in research. Understanding what made the experiment failed was more important. Using data analysis, researchers can gain a better understanding of their project. With a better understanding, they are better equipped to tackle the various problems they encounter. A proper and clear diagram displaying the experimental data is essential to prove the reliability and credibility of any research project. Therefore, experiments must be done with utmost accuracy to obtain credible results. For my future projects, I will definitely stress the importance of data analysis and ensure that the accuracy of collecting data must not be overlooked.

By sitting in the various meetings, I have gained a better understanding of how a researcher thinks. This taught me to expand my thinking and brainstorming skills when faced with difficulties. Patience and passion are needed to excel as a researcher. With patience, one can stay calm throughout this long and tedious process of many trials and errors. With passion, the researcher will always be finding new solutions to problems in hopes to improve many lives. A single issue may have been dealt by many researchers and with many approaches. Therefore, researchers are challenged to think outside the box and use their creativity to come up with different and unique innovations to solve such problems. Like researchers, as biomedical engineers, we are also taught to be problem-solvers to help improve the healthcare industry to better the lives of many.

During the course of my internship, I had the opportunity to interact with colleagues from different backgrounds, countries, and cultures. To be respectful towards their culture, I made sure not to ask or say anything that may offend them. As I interacted with them, I learnt about their different traditions, dialects, and cultures and share mine. In hopes to keep the inclusive and professional environment, I tried to avoid probing into any sensitive areas and making sure to never give in to stereotypes. With the help of the other scientist, I was able to adjust to the company’s work ethic.

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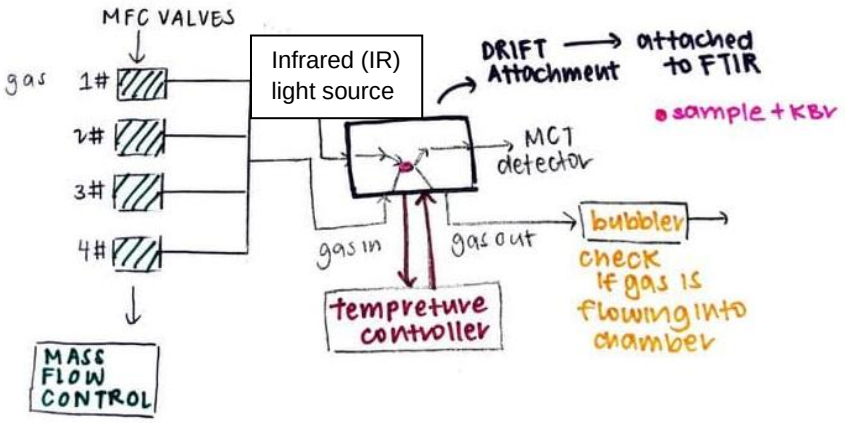
As Singapore went back to phase 2, ICES had to work in split teams. Unlike some of my friends, I was fortunate enough to still be able to work in the lab on alternate weeks and not entirely from home. Conducting experiments alone allow me to develop useful skills like independence and time management. Without Xiao Xin there to guide me, I found myself slowly gaining the confidence to conduct various experiments on my own. Given a deadline to meet, I gradually learn to complete multiple tasks all at once. Before going to the lab, I wrote out the various tasks I had to complete by the end of the day and the order to go about finishing them. I had to consider many factors such as the preparation, collection, ageing time and even the time taken for the oil bath to heat up. Before working in split teams, my schedule for the day depended on what Xiao Xin needed me to do. Therefore, working by myself allowed me to maximise and take charge of my time. Similarly, when I was working from home, I had ample time to broaden my knowledge on the projects and the various instruments used in the lab. This will allow me to take the necessary precaution or understanding when using the instruments in the lab. With more knowledge, I would not be following instructions blindly and may even be able to troubleshoot instruments independently when I was faced with a problem.

In conclusion, this internship has been a very fruitful one filled with many first-hand experiences. Through this work experience, I was able to develop communication, problem-solving, time-management skills, build teamwork, and learn the art of multitasking. These lessons are so valuable and cannot be taught using a textbook. As I continue my studies and enter the working world, I will apply the many valuable lessons I have gain throughout the past 22 weeks.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Appendix A1 DRIFTS experiment setup



Appendix A1-1: DRIFTS Set-up

The DRIFTS experiments aimed to observe the transformation of reactions occurring on the surface of various samples (catalysts). To achieve that, a controlled environment was created using multiple instruments as shown in the figure above. This set-up will allow the researchers to manage the various parameters, such as gas reactants flowrates or temperature of the chamber, that will affect the experimental results.

FTIR Spectrometer

Appendix A1-2: FTIR Spectrometer

(Perkin Elmer, n.d.)

FTIR spectrometer makes use of an infra-red (IR) light source and a Mercury-Cadmium-Telluride (MCT) IR detector. An MCT detector is a thermoelectrically cooled semiconductor containing electrons that absorb the electrons from the reflected IR light to generate an electrical current. To prevent overheating of the

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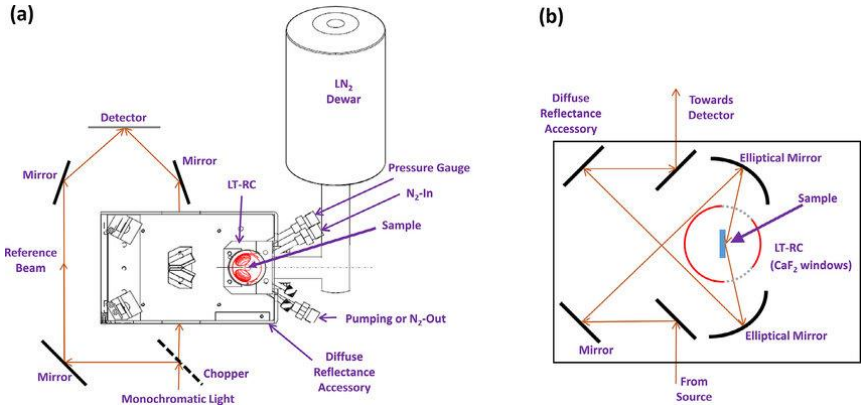
MCT detector and to obtain a stable detector performance, liquid Nitrogen is needed to keep the environment around the detector cool. Nitrogen has a low boiling point and therefore at liquid state, its' temperature is very low (− 196 °C).

Appendix A1-3: DRIFTS attachment

(Thermo Fisher Scientific Logo, n.d.)



Appendix A1-4: Light path in the chamber

(Bu, et al., 2017)

Appendix A1-3 is the attachment used to direct the IR light onto the sample to allow diffuse reflectance of the IR light to occur in the sample. Potassium Bromide, KBr is used as an IR transparent matrix to allow the light to reflect freely. Therefore, KBr was loaded with the sample to promote diffuse reflectance occurrence. Appendix A1-4 displayed the light path from the IR source to the sample and into the MCT detector. Inside the chamber, there are six mirrors strategically placed to reflect the IR light from the light source and onto the sample as well as reflect the reflected light

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from the sample into the detector. The light will be shone onto the sample at a range of wavelengths (4000 to 400cm^{-1}), and a spectrum is then produced and displayed on the FTIR software.

Mass Flow Controller

Appendix A1-5: Mass Flow Controller

(Geminibv, n.d.)

A Mass Flow Controller (MFC) is used to fully open and close the valves or manually control the flow rate of the gases passing through the valves. The concentration of specific gas reactants in a gas mixture or the exposure of the sample to the unreacted gas reactants can be managed when purged into the DRIFTS chamber. Refer to Appendix A2 for the experiment followed to test the accuracy of the MFC.

Temperature Controller

Appendix A1-6: Temperature controller

(Harrick Scientific Products, Inc., 2016)

The temperature controller shown in the figure above can be manually programmed to control and maintain the temperature of the DRIFTS chamber. Along with an external heater and sample thermocouple, the controller is attached to the FTIR

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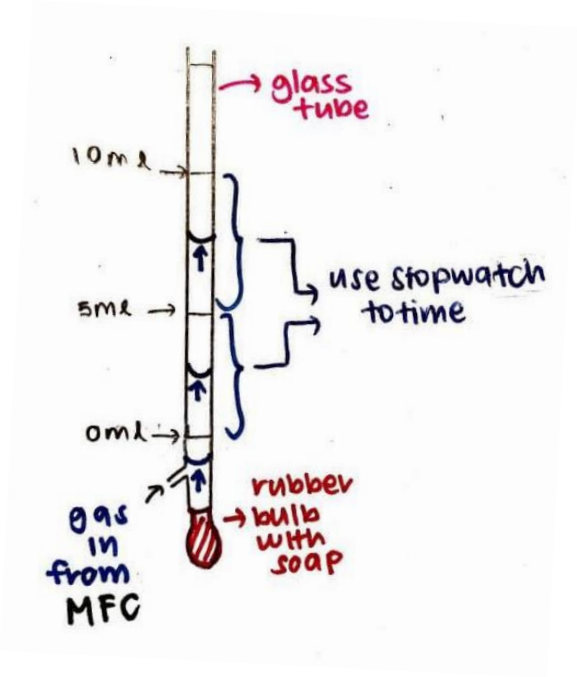
spectrometer along with an external heater and sample thermocouple. During experiments, the temperature of the chamber can be kept at optimum temperature using this controller. There are two temperature sensors inputs and one low-voltage output that is connected to the heater.

Two set points must be inputted. One controls the temperature of the sample while the other is a safety feature to prevent the chamber from overheating. When the chamber reaches the second set-point temperature, the device is immediately turned off.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Appendix A2 Testing Accuracy of MFC



Appendix A2-1: Drawn set-up of the experiment

A glass tube was held vertically upright using a retort stand. The bottom left side of the glass tube was attached to the output of the Mass Flow Controller (MFC). A rubber bulb was then attached to the same end of the glass tube as the MFC.

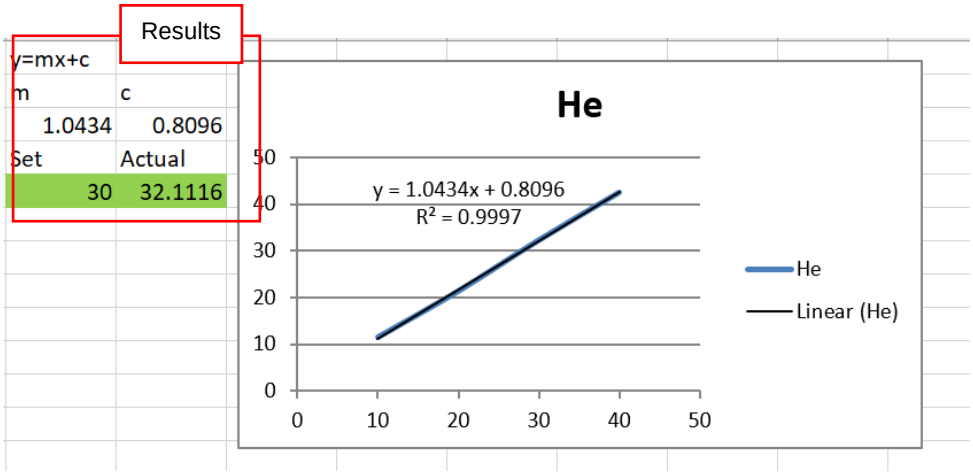
Procedure

When one of the MFC valves was open and the gas flows into the glass tube and a bubble ring was formed. As the gas was being blown into the tube, the bubble would continue to travel up. The flow rate displayed on the MFC is measured in ml/min. Hence, by recording the time taken for the bubble to reach the 5ml mark and the 10ml mark on the glass tube, the actual flow rate of the MFC could be calculated. This experiment was repeated for the 4 different gas reactants and at 4 different displayed flowrates for each gas (10ml/min, 20ml/min, 30ml/min and 40ml/min).

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

He	ml	1st	2nd	Average	Resullts	Average	Flowrate		Set	Actual
10ml/min	5	26.25	26.16	26.205	0.190803	0.190242	11.41454		10	11.41454
	10	52.85	52.59	52.72	0.189681				20	21.33575
20ml/min	5	14.16	13.49	13.825	0.361664	0.355596	21.33575		30	32.28036
	10	28.58	28.64	28.61	0.349528				40	42.54565
30ml/min	5	9.47	8.89	9.18	0.544662	0.538006	32.28036			
	10	18.77	18.87	18.82	0.53135					
40ml/min	5	7	7.1	7.05	0.70922	0.709094	42.54565			
	10	14.26	13.95	14.105	0.708968					

Appendix A2-2: Helium (He) results from flowrate experiment



Appendix A2-3: Graph of Helium (He) results

Using the data collected, a graph of the displayed flow rate against the actual flow rate could be plotted. This graph and its' equation as seen in Appendix A2-3 could then be used to calculate and set the accurate flow rate for the gas reactants for future experiments.

Importance

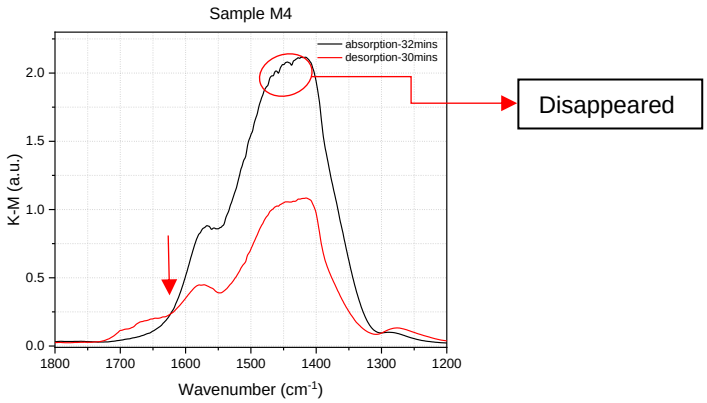
This experiment was important as it helps to minimise instrumental error when conducting the DRIFTS experiments. It allowed the researcher to set the accurate flow rate and percentage of the different gas reactants flowing into the chamber. Therefore, producing more reliable and accurate experimental results.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Appendix A3 Plotting of DRIFTS Graphs

Using a feature on the FTIR spectrum software, the background was subtracted from the selected spectra and the unit was converted to either Absorbance or Kubelka Munk (K-M). K-M is a unit used to measure the amount of diffuse reflectance that occurs. Whereas Absorbance is used to measure the amount of light that the substance absorbs at a specified wavelength. The unit used depended on the strength of the diffuse reflectance occurring in the sample. This will be further touched on in a paragraph under section 2.5 “Challenges Faced”.

Stepwise:

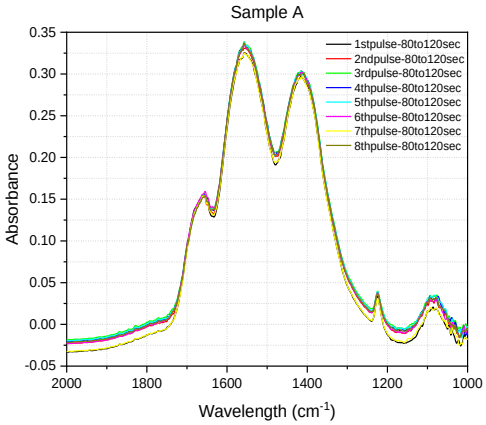


Appendix A3-1: Absorption and Desorption graph of sample M4

The desorption and absorption spectra of gas reactant A were plotted against each other. This was to observe which peaks remained, disappeared, or decreased. The remaining peaks would indicate the absorbed material could not be removed from the surface of the sample. Those peaks that disappeared or decreased as seen in Appendix A3-1 suggest that those materials were either physically absorbed by the sample, were gas-phase or both.

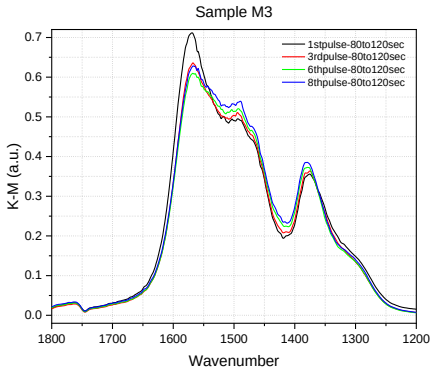
Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Procedure 1 (pulsing):



Appendix A3-2: Pulse graph of sample A

Besides the absorption and desorption spectra, the pulse spectra were also plotted on a separate graph. At first, the 80 to 120 seconds spectrum of each pulse were plotted together. Although this displayed a more gradual breakdown of the transition of reactions, it can cause the graph to be very messy and hard to read due to overlapping peaks.

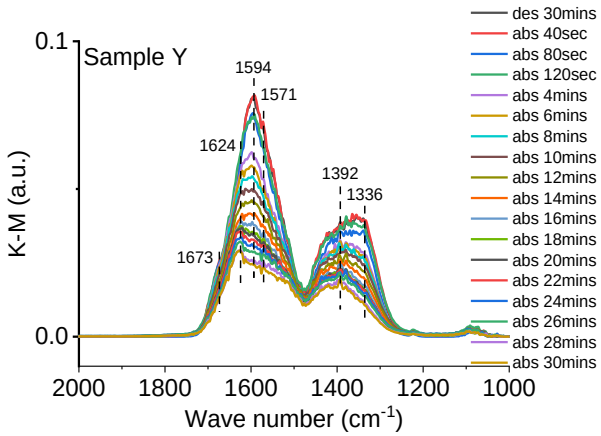


Appendix A3-3: Pulse graph of sample M3

Therefore, the 80 to 120 seconds spectrum of the 1st, 3rd, 6th, and 8th pulse were used instead. The graph was a lot neater making it better for comparison. The transformation of reactions could be observed a lot easier.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

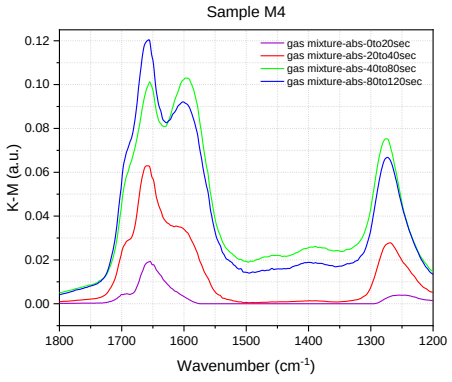
Procedure 2 (Continuous Flow):



Appendix A3-4: Sample Y stepwise spectra

In Appendix A3-4, all the gas reactant B absorption spectra were plotted together along with the last desorption spectra. Gradual change between the graphs could be seen as all the spectra had very similar shapes. Thus, although the spectra overlapped, the changes between the graphs were still very clear as the overlap was little. Having the spectra so close together also allowed for easier comparison between the spectra. Changes observed for small peaks were a lot more distinct and the presence of “shoulders”, labelled at 1673 cm-1 in Appendix A3-4, were also more prominent.

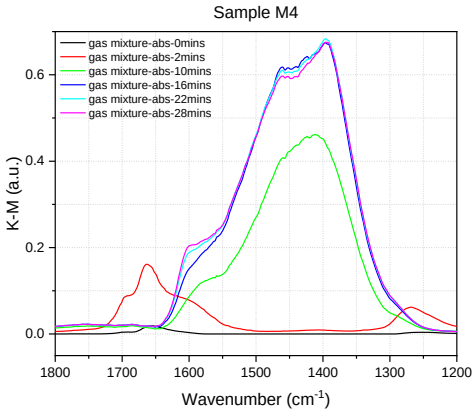
Mixed Gas:



Appendix A3-5: First 2minutes of absorption graph of sample M4

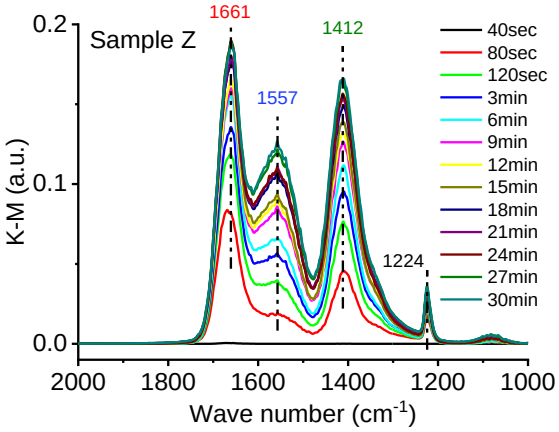
As seen in Appendix A3-5, the spectra obtained from the first 2 minutes were plotted together.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.



Appendix A3-6: Absorption graph of sample M4

At first, all the other spectra obtained within the 30minutes were plotted against each other. Only six out of all the spectra were plotted using Origin as shown in the figure above. These spectra showed distinct changes and thus, displaying a clear transition of the reactions that have occurred on the surface of the sample.



Appendix A3-7: Sample Z Mixed Gas Spectra

When testing a new type of catalyst, this format and aesthetic of the spectra were later altered to better display the data and observation of the experiment. All the absorption spectra were plotted together to get a more gradual change between each interval. Since the changes between the spectra were very minimal, having the spectra side by side ease the observation of such changes in smaller peaks and disappearing shoulders.

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Appendix B1 Calcination

Calcination is a process that heats a concentrated ore such as a carbonate or hydrated oxide at a very high temperature to remove any volatile substances, making the sample friable, or to oxidise a specific mass. It can be used as a form of “purification”.

Appendix B1-1: Samples loaded into Furnace

The solid catalysts were poured into ceramic bowls to be placed in the chamber furnace to undergo calcination. Labelling the catalysts was an important step to prevent any mix up from happening. This may occur as the colour of the catalyst may change after calcination, therefore making it harder to distinguish which catalyst is which.

Appendix B1-2: Chamber Furnace (Fisher Scientific , n.d.)

The catalysts were calcined using a Chamber Furnace as shown above. The chamber has numerous features that must be set before the samples were calcined. Firstly, the desired temperature that the sample would be calcined at had to be specified along with the heating rate which is measured at degrees per minute. Next,

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

the holding time must be set. This is the duration the furnace temperature will be held at the desired temperature.

One important precaution that had to be taken was to shut the furnace lid slowly and carefully. If the lid was shut forcefully, tiny black flakes of contamination will chip off from the top of the furnace and fall into the ceramic bowls. This will lead to obtaining contaminated samples in which will affect the accuracy of the experimental results. Refer to Appendix B2 for testing of catalyst performance and B3 for testing of chemical composition.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Appendix B2 Testing Catalyst Performance

There are 3 things to take note of to determine a catalyst performance. Firstly, the activity of the reaction. This refers to the conversion rate of the reactants to the products. Next, the selectivity, which represents the amount of desired product obtained from a certain amount of reactant. Lastly, the stability which is an indication of the amount of desired product that remains unchanged and would not convert back into its' reactants or the intermediate species or to other undesired products after a long time.

Procedure

Appendix B2-1: Hydraulic Press

(Mineral Innovative Technologies, n.d.)

Appendix B2-2: Strainer

(Science First, 2011)

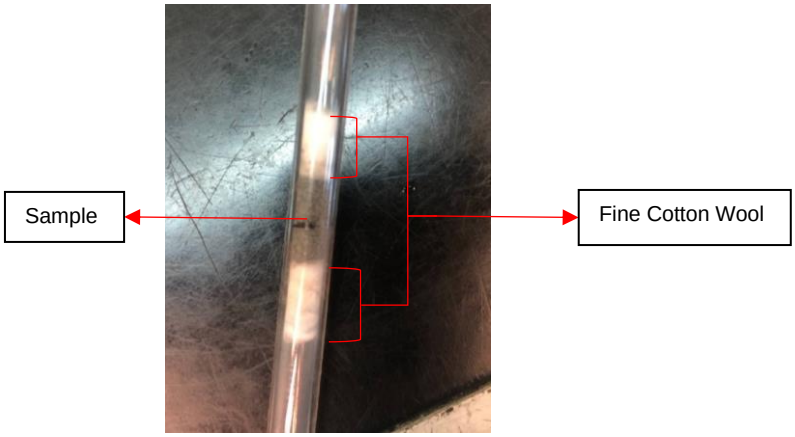
Using a hydraulic press, the sample was compressed to increase its particle size. Once the sample was compressed, the large, flattened pieces would be crushed and strained using a strainer as shown in Appendix B2-2. The different grid size for each

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

level of the strainer allows the sample with the desired particle size to be separated out. The sample with the desired size will be collected and poured into a small storage test tube.

Appendix B2-3: Desired particle size of sample

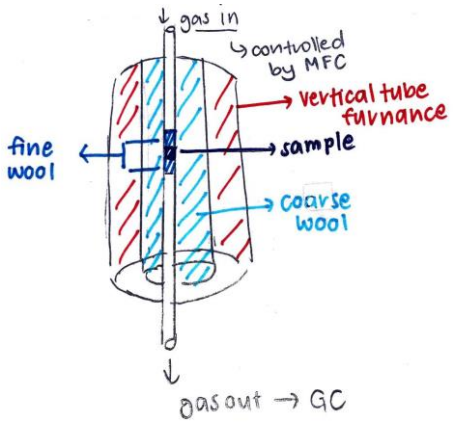
The sample particle size plays an important role when ensuring efficient reactions can take place. If the sample remained as a powder, there will be very few air spaces between the particles. Therefore, limited gas reactants will be able to flow through and the reaction cannot occur efficiently. If too big, the air spaces between the particles are too large making the reaction contact time too short.



Appendix B2-4: Glass tube with sample

After the sample with the desired size was collected, a glass tube had to be prepared as shown in the figure above. Firstly, a line had to be drawn on the glass tube to mark the centre of the reactor. Fine cotton wool was then pushed into the tube until it is slightly under the marked line. Next, 200mg of sample was weighed and then poured into the tube. Half of the sample must fall below the marking. Lastly, more fine wool was used to seal the other end of the glass tube. This created a fixed bed that supported the sample.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.



Appendix B2-5: Set-up of reactor

The glass tube was then loaded into the reactor where the gas reactants will flow through the tube to undergo a chemical reaction in the presence of the sample which was a catalyst.

Another important factor to take note of when conducting this experiment was that the airflow of the gas reactant must be just right. An MFC was used to control the flow of the gas reactant into the glass tube. If it was too slow, it may lead to the products or intermediate forming on the outer surface of the particle. If the particle becomes fully enclosed by the product or intermediate, it will lose its' reactivity. If too fast, this will cause turbulence, all the reactant particles will overcome resistance leading to a short reaction contact time.

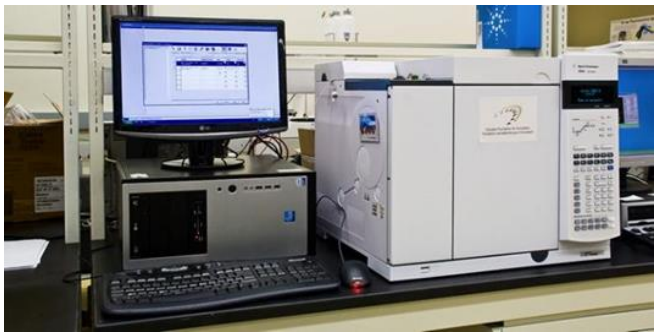
Appendix B2-6: Vertical Tube Furnace

(Norrscope, n.d.)

Coarse wool was used to fill up the air spaces between the glass tube and the vertical heating furnace. Coarse wool is a better conductor of heat than air, hence was used to ensure the reaction in the glass tube took place at optimum

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

temperature. The difference between coarse wool and fine wool is that fine wool has a smaller diameter and is a poorer conductor of heat than coarse wool.

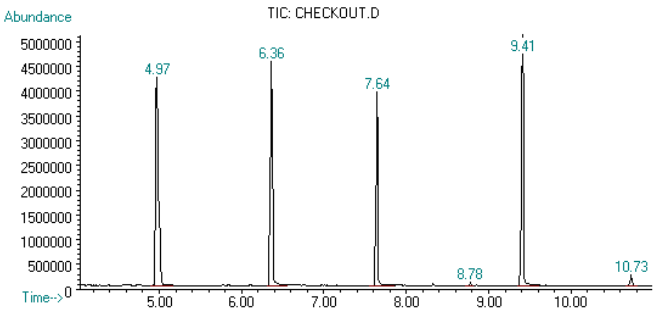


Appendix B2-7: Gas Chromatography

(Western University, n.d.)

A gas chromatography instrument was used to measure the presence of gas products produced in the glass tube and its' concentration. GC utilises the different gas's volatility to separate and differentiate the gases. As the gases leave the glass tube and enter the GC, it passes through the analytic column made of stationary phase materials. The mobile phase gases will interact with the stationary phase. Depending on their interaction, the various gases present will flow out of the column in a specific order. A detector is then used to detect the presence of any analyte molecules found in the elute. During this process, a GC chromatograph is produced. This spectrum will be taken at different temperatures and timings.

Data analysis



Appendix B2-8: Sample GC spectrum

(George Mason University , 1998)

Once all the chromatographs were completed, the area enclosed by each peak was measured and compared between the different temperatures. This helped the

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

researcher identify which temperature a certain gas product was most present. Therefore, the temperature at which the sample was the most reactive can be determined.

The area under each peak was used to calculate the conversion rate, selectivity of the catalyst and the yield of the desired product produced. If these calculations are greater than that of when no catalyst was used, it can be concluded that the catalyst was effective. However, if it is lesser than or equal to, the catalyst was not effective. All these data will be recorded and calculated using Excel.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Appendix B3 Testing of Catalyst Composition

X-ray diffraction analysis (XRD)

Appendix B3-1: XRD instrument

(Geochemical Instrumentation and Analysis, n.d.)

Concepts:

XRD is a technique used to determine the presence, amounts, and species of minerals in a sample. More specifically, XRD is used to identify the crystallographic structure and phase of this material. It does this by irradiating X-rays into a material. Known as elastic scattering, these X-rays will be scattered by interacting with the crystal atoms' electrons and produce spherical waves in multiple directions. Through destructive interference, these waves will cancel out each other. However, they will also add to constructive waves scattered in a few directions. These waves are then measured, and the diffraction pattern of the waves is used to identify the elements present in the sample.

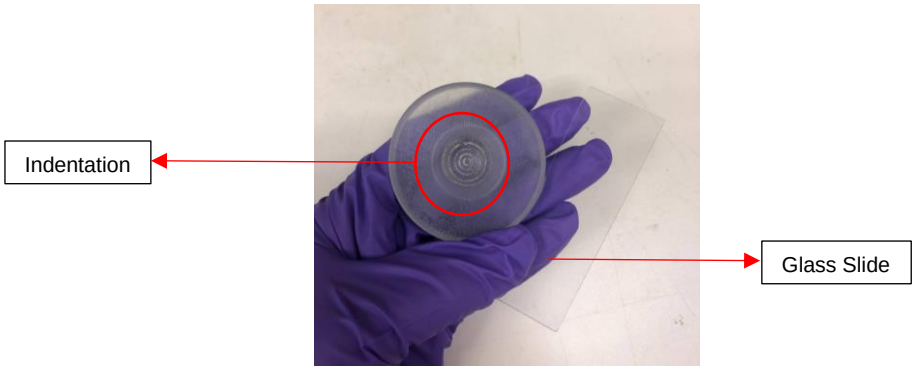
There are two types of identifications, phase and peak. Phase identification allows the XRD to determine the difference between the actual and ideal structure of the material using internal stresses and defects. Whereas peak identification aids with identifying the elements found in the sample. To determine the phase of the sample, the pattern observed on the measured spectrum is compared with the patterns entered in the reference databases of the XRD using a search-match algorithm. The pattern is determined by the peak position and intensity at a given wavelength.

For peak identification, the individual peaks are separated from one another and compared with reference peaks for identifications. This can either be done

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

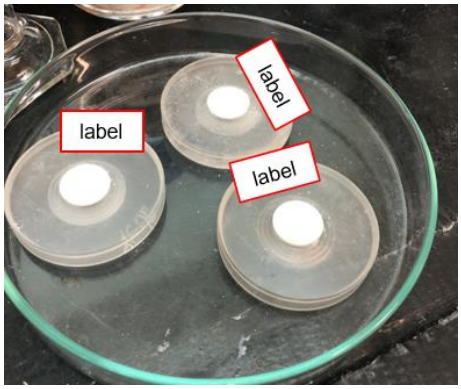
automatically or manually. There are a series of steps taken to ensure that peak identifications are done accurately. After the peaks are separated, the background spectrum is subtracted from the measured spectrum. The presence of amorphous phases and air scattering creates a significant amount of background which can interfere with the data analysis. The next step is to smooth the peaks to remove the random noise signals picked up with the desired peaks. Peak identification occurs during this process. Once identified, a profile fit is done to refine the peak positions and intensities.

Sample preparation for testing:



Appendix B3-2: XRD Specimen Holder and Glass Slide

The powdered sample was poured into the circular indentation located in the centre of the specimen holder as seen in Appendix B3-2. Using a glass slide, the powder was pressed ensuring that the whole indentation was filled as shown in the figure below. Once filled, the glass slide was then used to smoothen the top of the powder and remove any excess powder.



Appendix B3-3: XRD specimen holder with specimen

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

How calcination affects XRD spectra:

Before being calcined, some of the powdered samples were spared to be tested using the XRD. Once calcined, the calcined samples will also be tested. Testing the sample before and after calcination helps the researcher to better understand the sample by identifying the phase of the precursor and the transformation that occurs in that specific sample. Research shows that the higher the calcination temperature, the sharper, narrower and higher the intensity of the diffraction peaks. (Gharagozlou, 2011). The width of the peaks helps to determine the sample's crystallite size. Therefore, the narrower the peaks, the bigger the sample's crystallite size and the higher the crystallinity of the final product.

X-Ray Fluorescence (XRF)

Appendix B3-4: XRF Instrument

(Bruker, n.d.)

Concepts:

XRF is a technique that uses X-ray beams to displace electrons from their orbital positions in an atom, releasing a burst of energy that is specific to an element. This energy characterizes the chemical composition found in an unknown sample without determining the elements' phases. An atom consists of electron shell(s) which contain electrons surrounding a nucleus made of protons and nucleons. An x-ray beam of enough strength to displace the electrons on the inner orbital shells of the atom is emitted from the analyser. For this displacement to happen, the energy of the emitted X-Ray beam must be higher than the binding energy holding the electrons at their fixed positions. When the electrons leave their orbital positions, vacancies are formed causing the atom to be unstable. To correct this instability, the atom must immediately use an electron from a higher orbit to fill in these vacancies. This process is known as fluorescence. As the electron moves from a higher shell to

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

a lower shell, it loses and releases energy, known as fluorescent energies, of different strength depending on the distance between the electron shells. This distance is unique to each element. The individual fluorescent energies, specific to each element present in the sample, are detected. The quantity of each element found in a sample can be determined by measuring the amount of detected individual fluorescent energies of that desired element.

Inductively coupled plasma-optical emission spectrometry (ICP-OES)

Appendix B3-5: ICP-optical emission spectrometer

(Technology Networks, 2020)

ICP-OES is used to analyse the major and trace elements found in a sample. The probe of the autosampler as seen in Appendix B3-5 in the spectrometer draws the sample from the storage tube and into the nebulizer where the liquid sample is converted into a mist of tiny droplets. This mist will then be introduced to the torch which consists of a chamber containing argon gas and surrounded by an electromagnetic coil. When the electromagnetic coil induces a magnetic field, a plasma is formed. The sample enters the plasma exciting its' electrons to a higher state. As the electrons return to its' normal state, energy is released in the form of light. The lights emitted by the different elements are separated using a group of pistons to aid in identification. The light is then captured by cameras placed at different angles. The cameras record the wavelength at which the light is emitted and the intensity of each light. The wavelength will allow the researchers to determine the different elements present in the sample. Whereas the intensity at the different wavelengths helps in the computing of the concentration of that specific element in the sample.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Nuclear Magnetic Resonance (NMR) spectrometer

Appendix B3-6: NMR instrument

(Bruker, n.d.)

Concept:

NMR seen in the above figure is used by researchers to study the physical, chemical, and biological properties of a material to identify its' molecular structure in detail. The nuclei of the atoms in a material are exposed to radio waves. Certain atomic nuclei contain protons which are positively charged particles that spin. Spinning charged particles will generate a magnetic field. The overall magnetic fields of each proton are pointing in random directions.

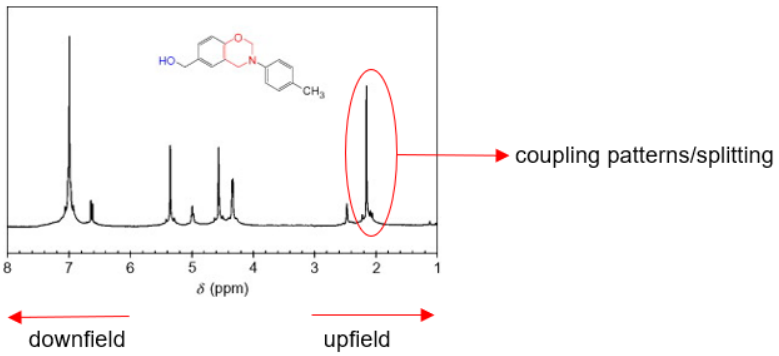
When these protons are subjected to a strong external magnetic field, its' overall magnetic field will either point in the opposite or the same direction as the external magnetic field. These two directions indicate the two energy states of the proton. The high-energy state proton creates a magnetic field that opposes that of the external magnetic field. Whereas the low-energy state proton produces a magnetic field in the same direction as that of the external magnetic field.

These protons are then bombarded with radiofrequency radiation at different wavelengths. If the radio waves are at the appropriate frequency that matches the energy difference between the high and low energy states, a spin-flip can occur. This is when the protons absorb these radio waves and flip so that the magnetic field is going from aligned to opposed or opposed to aligned. As the proton moves from its excited state back to its normal state, the absorbed radio waves are emitted and measured. This feedback is known as resonance.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Data analysis:

The difference between the two spin states varies depending on the number of protons or neutrons located in the nucleus of an element. This number is unique to each element. Therefore, by comparing the measured spectrum to the spectral libraries, researchers can determine the elements located in the sample. There are three things to take note of when interpreting an NMR spectrum.



Appendix B3-7: NMR spectrum

(Ishida & Agag, 2011)

Firstly, it is the chemical shift that helps to differentiate elements with nuclei of the same kind but are in different chemical environments. Chemical shift refers to the location at which the peaks appear on the measured spectrum, either up or downfield. The two factors affecting chemical shifting is deshielding and anisotropy. The electron surrounding the nucleus produces an induced magnetic field that opposes that of the protons. The induced magnetic field shields the protons from the external magnetic field. This reduces the impact of the external magnetic field experienced by the proton and thus, lesser radiofrequency is required for the spin-flip.

In the presence of electronegative groups, the electron density of the surrounding nucleus decreases as deshielding occurs. Therefore, the more external magnetic field is experienced by the protons and thus more radio frequency is absorbed causing the chemical shift to increase downfield.

Anisotropy occurs due to the spinning of the protons of a certain group of compounds known as the pi system. When exposed to the static magnetic field, these protons will spin producing a third magnetic field. This additional magnetic field

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

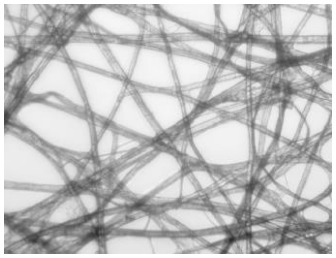
results in either more or less shielding of nearby protons depending on its relative position to this field. The higher the shielding, the lower the magnetic field experienced by the protons. Therefore, the chemical shifts more up field as a lower radio frequency is needed to achieve a spin-flip.

Secondly, the integration helps determine how many chemically equivalent protons are generating that peak. The integration refers to the area under a peak. It can be used to find the concentration of each element found in the sample.

Lastly, it is coupling patterns. Chemically equivalent protons will produce the same resonance, but that resonance is split into a certain number of smaller peaks. This number is dependent on the neighbouring protons. When the resonance of a proton encounters the magnetic field of the neighbouring protons, the resonance signal will be split into n + 1 smaller peaks, n being the number of neighbouring protons. By counting the number of smaller peaks present, the researcher can find the number of neighbouring protons that surround a specific proton.

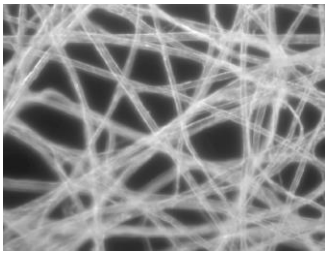
All these factors in the spectrum can help the researcher to determine the elements present and the structure of the unknown sample.

Transmission Electron Microscope (TEM)



Appendix B3-8: TEM sample under bright field

(Gaston & Le, 2020)



Appendix B2-9: TEM sample under dark field

(Gaston & Le, 2020)

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

A TEM is a microscopy technique that involves passing a beam of electrons through a specimen to produce an image. The specimen is usually ultrathin, and thickness is lesser than 100nm. The image is formed due to the specimen's interaction with the electrons. TEM magnifies objects by at most 2 million times.

There are two different modes, dark and bright field mode. The bright field mode captures the whole image at once since the electron beam is shone onto the whole sample. Whereas, under dark field, the electron beam is focused on certain areas of the sample at one time. Heavier elements found in the sample will appear darker in the bright field but brighter in the dark field. Heavier elements can absorb and scatter more electrons than lighter elements causing them to appear darker under the bright field mode. However, using a dark field mode, the scatter electrons of the heavier elements are selected instead and therefore appearing brighter. The dark field mode allows the researcher to obtain a more visually appealing image as it helps to enhance contrast. The captured image can be used in research papers to display the structure and composition of the sample.

A TEM can also be used to identify the different elements found in a certain area of the sample. Under the dark field mode, there are detectors located in the TEM that will help to detect whether the desired element is present and its' specific location with a selected area. This will help the researcher test the purity of the sample and thus increase the credibility of the experimental results.

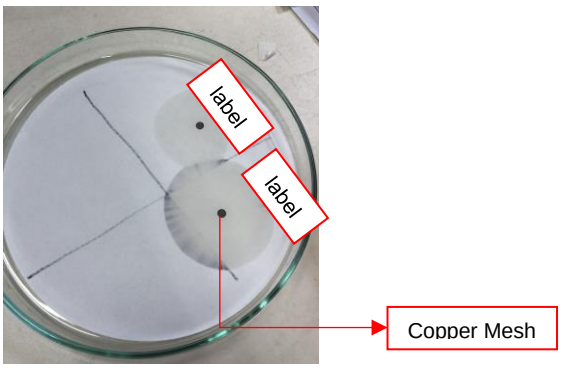
Sample preparation for testing:

A mixture of the solid sample and a solvent, normally ethanol, must be prepared. A small amount of the sample was poured into a narrow glass bottle. Ethanol was then used to fill up the rest of the bottle. The bottle was capped and placed into an ultrasonic cleaner as shown below.

Appendix B3-10: Ultrasonic Cleaner (DKSH, n.d.)

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

An ultrasonic cleaner is a homogenizer used to break up the molecular bonds to allow two substances to be thoroughly mixed. When a solvent is exposed to high-frequency ultrasonic waves, vacuum bubbles are formed due to the alternating high and low pressure. As these bubbles grow and merge with each other, they will eventually become too big and burst. This process is known as cavitation. Cavitation will result in sending of shock waves through the mixture. The presence of such shock waves and the vibrations created by the ultrasonic cleaner will disrupt the surrounding covalent bonds of the solid sample. The mixture now consists of solid samples broken up into nanoparticles that are dispersed within the solvent.



Appendix B3-11: TEM specimen preparation

A filter paper was divided into four sections each for one sample. Depending on the number of samples tested, the sections were labelled, and a small copper mesh was placed in each labelled section. A disposable pipette was then used to add 2-3 drops of the prepared mixture onto each mesh. The samples are then left to air dry before TEM imaging.

A typical TEM grid consists of a flat disc with a mesh or other shape holes. They are used to support a thin layer of the sample. The presence of such holes helps to allow the electrons to pass through. TEM grids come in various shapes and materials which are used for different applications. The material of the grids is chosen based on the specimen used. Some specimens will react with certain materials while others may require a high-temperature analysis. To prevent the sample from falling through, additional support can also be provided on the top of the girds. An example would be applying a carbon coating across the surface of the sample to provide the necessary support without significantly disrupting the flow of electrons.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Scanning Electron Microscope (SEM)

Appendix B3-12: Scanning Electron Microscope

(Earth Observatory of Singapore, n.d.)

SEM is a microscope that scans the surface of samples in a raster-like pattern using a focused electron beam to produce magnified images. Various signals, scattered electrons, will be produced as the electrons interact with the atoms of the sample. These signals are then detected and used to determine the sample's surface topography and composition. Like the TEM, the SEM has a function that can identify the elements present on a captured area of the sample's surface. However, SEM produces a clear and detailed image of the sample's surface which a TEM is unable to provide.

Splutter coating is needed to help to increase the conductivity of the sample surface. If the sample surface is nonconducting, there will be a build-up of electron charge that will lead to obtaining blurred images. An ultra-thin layer of an electrically conducting metal will be applied to the sample to improve the image resolution.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Appendix C1 Code of Random Guessing Game

```
import random


#generate new num
def randnum():
    y = (level*100)+1 #increase difficulties
    global num
    num = random.randrange(y)
    print('Start playing LEVEL %d' %level)
    global i
    i = 0

level = 1
ts  = 'Your score is {}'
score = 0
x = 'y'

while x.upper() == 'Y':
    randnum()
    while i<8:
        user = input('Enter your guess:')
        if(user.isnumeric()):
            user = int(user)
            if (user<0 or user>level*100):
                print('Invalid input!! Please keep within the range')
            else:
                if (user == num): #user input matches
                    score = score + 1
                    print('Correct! ' + ts.format(score))
                    level = level + 1
                    randnum()
                else:
                    if (user>num):
                        print('Too high! try again')
                    else:
                        print('Too low! try again')
                    i = i + 1
        else:
            print('Invalid input! Please input an integer!')

    print('Game Over! ' + ts.format(score))
    score = 0 #restart score
    level = 1
    x = input('Do wish to play again?(Y/N)')
```

Appendix C1-1: Random Number Guessing Game Code

The function “randnum()” was made use of the “random.randrange()” command to generate a random number that is stored in the global variable “num”. The use of this function helped to eliminate the need for repetitive commands which could make the code unnecessarily long and messy. The variable “y” controls the range of possible numbers that the player can guess for each level.

The global variable “i” measures the number of tries the player has taken. If the value of “i” exceeds 8, the while loop “while i<8” will return a false and the commands in the loop will no longer be executed. Therefore, the game will end and the user is prompted using the “input()” command if they wished to play again. This command was also used to obtain the player’s guess which was stored in the “user” variable.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

When the user inputs a valid number, the “user” variable is compared to the variable “num”. This process involves branches of if-else statements that will analyse and respond to the player’s guess accordingly. If the “user == num”, the score and level are increased by one and the “Correct…” statement is printed. The randnum() function is called to generate a new number for the next level. Since the level increase by one, the value of “y” is changed accordingly. If the “user>num”, the “Too High!” hint is printed. Likewise, if the user’s input does not meet the condition “user>num”, the “Too Low!” hint is printed.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Appendix C2 Code of Ordering System

```
import numpy as np
import datetime

x = 'Y'
order = []
cost = []
total = 0

bc = 10
sc = 5
dc = 2
mc = 15


menu = np.array([ ['Chicken Burger', 'Beef Burger', 'Fish Burger'], ['Fries', 'Nuggets', 'Salad'], ['Coke', 'Sprite', 'Fantagrape
# burger = menu[0]
# sides = menu[1]
# drinks = menu[2]

#menu
print("======= MENU =======")
print("Burgers($%d): " %bc + str(menu[0]))
print("Sides($%d):    " %sc + str(menu[1]))
print("Drinks($%d):   " %dc + str(menu[2]))
print("\n\nMeal option(includes burger, sides and drink): $%d\nStudents Discount(Weekdays only): 50%%" %mc)
print("==================")
#instruction
print("\nHow to order?\nKEY IN 0/1/2/3 for each the food\n0:None of the choices\n1:First choice\n2:Second Choice\n3:Third Choice\
```

Appendix C2-1: Code for Menu

In Appendix C2-1, various print statements were used to display the Menu as well as the instructions on how to order. A NumPy array “menu” was used to store the food options. The costs of one burger, side, drink and meal option were stored in the variables “bc”, “sc”, “dc” and “mc” respectively. The use of these variables helped to ease making any changes to the prices which aid when troubleshooting.

Numerous functions were created to make the program a lot neater by eliminating repetitive commands.

```
#include gst and service charge
def calculate(bill, sc, gst):
    return(bill*sc)*gst
```

Appendix C2-2: calculate() function code

The function “calculate()” was used to add the GST and service charge into the total cost of all the orders. It will be called at the end of the program when the bill is printed out. Variables “sc” and “gst” will be stated when the function is called as seen in Appendix C2-5.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

```
#store the order
def store(index1, index2):
    if (index2 != 0):
        return (menu[index1, (index2-1)])

#checking
def numeric(name, index, price):
    y = 0
    while (y == 0):
        user = input('Enter your %s order:' %name)
        if (user.isnumeric()):
            user = int(user)
            if (user>=0 and user<=3):
                if (user != 0):
                    global odr
                    global c
                    if (name == 'burger'):
                        odr = store(index,user)
                    else:
                        odr = odr + '\n' + store(index,user)
                    c = c + price
                else:
                    odr = odr + '\nNo ' + name
                print(odr)
                y = 1
                return user
            else:
                print('Please stay within the range(within 0 to 3)!!')
        else:
            print('Invalid Input!!')
```

Appendix C2-3: Functions used to interpret customer's input

The function ‘store()’ is used to read the customer’s input. It makes use of the various indexes to slice out the desired food choice in the NumPy array “menu” depending on the customer’s input. Variable “index1” selects the focused food option out of burgers, sides and drinks. Whereas “index2” is responsible for slicing out the chosen food choice of each food option.

Function “numeric()” helps to interpret the customer’s order and prevent the customer from entering any invalid inputs. Similar to the Random Guessing Game, the command “.isnumeric()” was used to ensure the customer’s input is an integer. To prevent the user from keying in a number out of range, an if-else statement was used. The global variables “odr” and “c” help to store the customer’s order and the cost of each order, respectively. As seen above, the value of “odr” changes with the addition of the customer’s most recent input. If the customer’s input is not equal to 0, the function “store” is called, and the selected food choice is added into the “odr” variable. However, If the customer inputs a 0, the addition will include a “No” followed by the focused food option. The while loop “while (y == 0) “ was implemented to prompt the customers to enter their food choice repeatedly until they input a valid number. This while loop is controlled by the variable ‘y’ and therefore the value y will only be changed to 1 when the customer’s input meets all the requirements.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

```
while (x.upper() == 'Y'):
    odr = ''
    c = 0

    b = numeric('burger', 0, bc)
    s = numeric('sides', 1, sc)
    d = numeric('drinks', 2, dc)

    #comfirm
    z = input('Would you like to confirm you order?(Y/N):')
    if (z.upper() == 'Y'):
        #order meal
        if ((b and s and d) != 0):
            meal = input('Do you want a meal?(Y/N):')
            if (meal.upper() == 'Y'):
                c = mc

        cost.append(c)
        order.append(odr)

    #more food?
    x = input('Order More Food?(Y/N):')
```

Appendix C2-4: Main Code

The while loop “(x.upper() == ‘Y’)” allows the customer to order multiple times. The while loop will only end when the customer inputs any other character apart from “y” or “Y” at the end of each order when prompt if they wished to order more food. At the start of the while loop, the variables “ord” and “c” are reset back to nill and 0, respectively. Their values will soon be altered using the “numeric()” function. The function is called once for each food option and the customer’s input is returned and store in one of the variables “b”, “s”, and “d” depending on the focused food option. If all three variables are not 0, indicating that the customer ordered one of every food option, the meal option will be provided using an “input()” statement. . If the customer goes for the food option, the cost of the order, “c”, will be changed to the cost of a meal which is specified at the start of the code. However, this meal option is only provided if the customer inputs a “y” or a “Y” when prompt to confirm their order. The customer’s input for this prompt is store into the variable “z” which controls the if statement used to store the variables “c” and “ord” in their respective string arrays. If the customer confirms their order, the values of “odr” and “c” will be added into the string arrays “order[ ]” and “cost[ ]” respectively. Each index in the array represents one order and therefore making it easy to distinguish between the orders. If the

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customer chooses to delete their order and order more food, the while loop will repeat and the values of “odr” and “c” will return to nil and 0.

```
#student discount
sm = 1
tdy = datetime.datetime.now()
if (tdy.weekday()<5):
    student = input('Are you a student?(Y/N):')
    if (student.upper() == 'Y'):
        sm = 0.5

print('\n~~~~~~~~~~~ BILL ~~~~~~~~~~~')
print(tdy)
for i in range(0, len(order)):
    print('\nOrder number #%d ==== $%s' %((i+1),cost[i]))
    print(order[i])
    total = total + int(cost[i])
print('\nTotal Amount              $%d' %total)
if (sm == 0.5):
    total = total*sm
    print('Student Discount          $%d' %(total))

total = calculate(total, 1.10, 1.07)

print('GST & Service Charge      $%d' %total)
```

Appendix C2-5: Student discount and Bill Code

The last part of the code helps to consolidate all the customer’s orders as well as calculate the cost. For the first section, the datetime64 library was used to determine if the day the customer orders their food is a weekday. The “.weekday()” command was used to produce a number between 0 to 6 depending on which day of the week it is. If the output of this command was less than five suggesting that it was a weekday, the student discount option will be provided. The program will change the value of the variable “sm” to 0.5 only if the customer inputs a “y” or a “Y” to the “Are you a student?” prompt. If not, the value of “sm” remains as one. The next section involves using a for loop to go through all individual stored values in the string arrays “order” and “cost”. As the value of “i” increases, each order is printed out along with its’ cost. The total cost is also calculated by adding all the values in the “cost[ ]” array. Once the total cost is calculated, the student discount is deducted followed by the addition of the GST and service charge. The “calculate()” function is called here. In between are various print statements that will print out the entire bill.

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

Appendix D Contact Information

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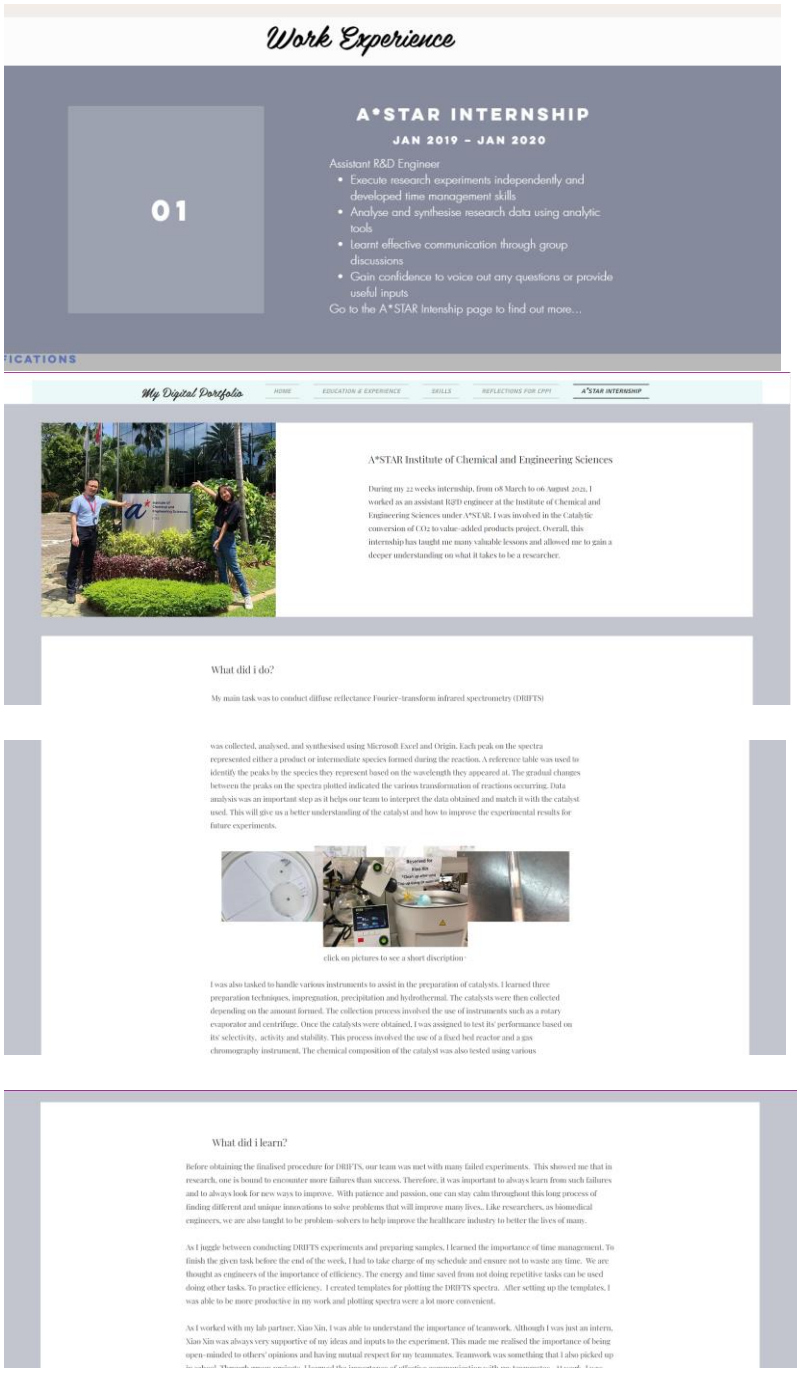
Appendix E Digital Portfolio



Wix Portfolio link:
https://s10192905.wixsite.com/website

Note: Due to A*STAR confidential policies, the information and pictures disclosed are limited.

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