IONS LIQUIDS AS POTENTIAL CO-CATALYST FOR CO₂ ELECTROCHEMICAL REDUCTION

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Abstract: Carbon dioxide electrochemical reduction (CO₂ER) presents numerous advantages in mitigating greenhouse gas emissions by converting CO₂ into value-added chemicals and can be integrated with renewable energy sources such as solar and wind. Nevertheless, establishing an electrochemically stable catalytic system that can effectively decrease the overpotential while maintaining high current density and faradic efficiency is challenging. The precise mechanisms causing the reactions and the specific functions of the electrode with electrolytes are still not fully understood. Hence, a significant increase in attention has been paid to using ionic liquids (ILs) as electrolytes for CO₂ER. This phenomenon is attributed to the unique capabilities of ILs to reduce overpotential, increase current density, and improve electrochemical stability. Therefore, this study evaluated the effect of incorporating ILs into electrolytes to comprehend the cation and anion influences on CO₂ER reactions. Linear sweep voltammetry (LSV) and chronamperometry (CA) were employed to examine the reduction peaks and current density values for different electrolytes, respectively. Consequently, a 0.1 M NBu₄PF₆ acetoniitrile solution containing 1-ethyl-3-methylimidazolium tetrafluoroborate [EMIM][BF₄] demonstrated a significantly lower onset potential of the reduction by 320 mV. A reduced CO₂ER efficiency involving ILs with long alkyl chains was also observed. Meanwhile, a novel hypothesis concerning molecular orbitals for the CO₂ER reaction mechanism was discussed. Overall, various performance variables (reduction stability, applied potential, and current density) of CO₂ER were improved using cations with short alkyl chains, anions with high highest occupied molecular orbital (HOMO) levels, and appropriate solvent media. These findings can serve as selection criteria to aid in choosing appropriate ionic liquids for CO₂ electrochemical reduction (CO₂ER).

Keywords: Ionic liquids, CO₂ conversion, electrochemical reduction, COSMO-RS, Turbomole

1. Introduction

Considering the progress of the global economy and society, the growing energy demand is a pressing issue that must be addressed. Despite the considerable advancements in green renewable energy sources (such as solar and wind energy), fossil fuels remain the dominant primary source (accounting for more than 80% of energy output) (Yang et al., 2008; Tian et al., 2022). Generally, fossil fuels release significant carbon dioxide (CO₂) into the atmosphere, causing its entrapment. Numerous environmental and climate change issues are then observed due to the disruption of the global carbon cycle. Higher sea levels and greenhouse effect intensification are two common examples caused by this phenomenon (Friedlingstein et al., 2014). Hence, the negative impacts necessitate a highly effective method for converting CO₂ into valuable compounds to lower the atmospheric CO₂ concentration. Several studies have addressed these issues by efficiently developing strategies to convert CO₂ into valuable carbon-based compounds. These approaches include thermal reduction (Shi et al., 2018), biotransformation (Karshima et al., 2024), photoelectrochemical (Bi et al., 2022), and electrochemical reduction (Gu et al., 2022).

The CO₂ electrochemical reduction (CO₂ER) system can produce numerous value-added products through CO₂ conversion, including methane (CH₄), ethylene (C₂H₄), carbon monoxide (CO), methanol (CH₃OH), formic acid (H₂CO₂), and ethanol (C₂H₅OH). Notably, the cathode material is the primary catalyst in the CO₂ER system. Multiple studies by Hori et al. also reported the effects of different metal catalysts on CO₂ER, such as Cu, Au, In, Sn, Pb, Zn, Ag, and Pd (Y. Hori et al., 1987; Y. Hori et al., 1994; Y. i. Hori, 2008). Consequently, Cu and its derivatives have been extensively researched as catalysts due to their unique capability to efficiently convert CO₂ into several higher products, surpassing the production of only CO. These reactions occur at ambient conditions and exhibit high current efficiencies. Nevertheless, ILs have garnered significant interest as an electrolyte for CO₂ER due to their distinctive characteristics,

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Received: February 7, 2024
Accepted: May 7, 2024
Published: July 31, 2024

DOI: https://doi.org/10.22452/mjs.vol43sp1.9
including excellent thermal and chemical stability, good CO$_2$ solubility, and the capacity to reduce the applied potential (Carlesi et al., 2014).

The cations of the ILs have been reported as the primary active component influencing catalytic performance and have garnered significant interest (Lau et al., 2016). Specifically, imidazolium-based ILs have demonstrated substantial potential and can be categorised into two divergent mechanisms. Firstly, the ILs and CO$_2$ form a covalent bonding by carboxylic adduct formation, or that hydride is transmitted. Secondly, the ILs and CO$_2$ form non-covalent interactions, such as stabilising complexes through alterations in the localised CO$_2$ environment or hydrogen bonding (Vasilyev et al., 2020).

A study by Aki et al. (2004) discovered that anions were crucial in determining the solubility of CO$_2$. The study also denoted that fluoroalkyl-containing anions (such as [TFSI] and [methide]) presented higher solubilities than other anions. Likewise, Snuffin et al. (2011) reported that [EMIM][BF$_4$] with a C$_3$ symmetric tetrahedral structure was more effective in electroreducing CO$_2$ compared to [BMIM][BF$_4$] and [BMIM][TFSI]. This outcome suggested a significant correlation between anion and catalytic performance. Nonetheless, insufficient studies have been observed regarding comprehending the precise reaction mechanisms and the distinct functions of cations and anions in electrochemical reduction reactions.

This study assessed the impact of different ILs on the CO$_2$ reduction peaks and current density values for two different CO$_2$ER setups. The molecular orbital energy levels [highest occupied molecular orbital (HOMO) and lowest occupied molecular orbital (LUMO)] of the various cations and anions were determined using a TmoleX simulation software. Furthermore, the impacts of the structure size and the HOMO value of the anion on the catalytic performance of CO$_2$ reduction were explored.

2. Materials and methods

2.1 Materials

The [BBT][BF$_4$], [BBT][TFSI], [BMIM][BF$_4$], and [BMIM][GLY] in this study were synthesised following the methods outlined in the authors’ previous article (Mohammed et al., 2022). Meanwhile, [EMIM][TFSI] (purity: ≥97.0%) and [HMIM][TFSI] (purity: ≥98.0%) were obtained from Sigma Aldrich without requiring any further purification. Figure 1 illustrates the structures of the selected ILs for this study.

2.2 CO$_2$ER setup

The electroreduction was conducted in an H-cell, in which an Ag/AgCl electrode was used as the reference electrode, and a Pt mesh of (1 cm × 1 cm) area was employed as the anode in 0.5 M H$_2$SO$_4$ anolyte solution. A Nafion 117 membrane was also utilised to separate the catholyte and anolyte to prevent the re-oxidation of the reduction products. This membrane underwent pretreatment through a series of three sequential steps: (i) pretreatment using 3% hydrogen peroxide for 1 h at 80°C, (ii) pretreatment using 0.5 M sulfuric acid solution for 1 h at 80°C, and (iii) rinsing process using distilled water. The purpose of this procedure was to cleanse the membrane of organic contaminants and protonation of the membrane (Navarra et al., 2008). A 0.5 L gas bag was also attached to the catholyte side to collect the gaseous products. Meanwhile, various ILs were introduced as additives into two distinct electrolyte systems based on the solubility of the ILs: (i) 0.1 M NaHCO$_3$ aqueous solution and (ii) 0.1 M NBu$_4$PF$_6$ acetonitrile (ACN) solution.

A) CO$_2$ER in NaHCO$_3$-aqueous based electrolytes

Five different electrolytes were studied as the catholyte, namely 0.1 M NaHCO$_3$-based electrolytes containing 0.02 M of four different ILs, including [BBT][BF$_4$], [BMIM][GLY], [EMIM][TFSI], and [BMIM][BF$_4$], alongside a 0.1 M NaHCO$_3$ solution without any IL. A copper (Cu) plate of 1 cm × 1 cm was used as the cathode, platinum (Pt) mesh as the anode, and Ag/AgCl as the reference electrode. The Cu plate was polished and cleaned using acetonitrile and water and then dried to eliminate particulate residue. Subsequently, N$_2$ gas was purged into the electrolytes for 15 mins. The pH of the selected electrolytes was then measured using a pH meter. Lastly, the electrolytes underwent a 40-minute purging process with CO$_2$, followed by an additional step of monitoring the pH before the CO$_2$ER reaction.

B) CO$_2$ER in NBu$_4$PF$_6$-based electrolytes

The cathode utilised in this part was a silver disc electrode with a diameter of 2 mm. Seven different catholytes were prepared namely 0.1 M NBu$_4$PF$_6$ acetonitrile solutions containing 0.02 M of six ILs including BBT][BF$_4$], [BBT][TFSI], [EMIM][BF$_4$], [EMIM][TFSI], [BMIM][BF$_4$], and [HMIM][TFSI]. A 0.1 M NBu$_4$PF$_6$ ACN solution without any IL was also employed as a reference.

2.3 Evaluation of reduction peak and current density

The CO$_2$ER reaction was assessed using a potentiostat (AutoLAB, PGSTAT128N) equipped with NOVA software. This study then used linear sweep voltammetry (LSV) based on a scan rate of 0.0049 V/s to determine the CO$_2$ reduction peak. Finally, a chronocoulamerometry (CA) method was used to conduct the reaction, depending on the reduction peak potential.
2.4 Molecular computational modelling study

A molecular computer modelling investigation was conducted using TmoleX to optimise the chosen structures and determine the LUMO and HOMO values of these structures. The TmoleX programme utilised parametrisation, incorporating triple-zeta valence with polarisation (TZVP) based on density functional theory (DFT). Typically, the sigma profile and sigma potential present extensive uses in determining the polarity of the molecule (Khan et al., 2023; Khan et al., 2020; Wojciechowski et al., 2021). Thus, these parameters were generated using COSMO-RS. The classifications of the parameters are as follows: (i) bond donor ($\sigma < -0.01$ e/Å$^2$), (ii) non-polar area for ($-0.01 < \sigma < +0.01$ e/Å$^2$), (iii) and hydrogen bond acceptor for ($\sigma > +0.01$ e/Å$^2$) (Klamt, 2005; Klamt, Jonas, Bürger, & Lohrenz, 1998).

3. Results and discussions

3.1 CO$_2$ER in 0.1 NaHCO$_3$ aqueous solution

Initially, the impact of introducing ILs on the pH of the CO$_2$ER system was evaluated. Table 1 tabulates the pH values for the selected electrolytes before and after purging CO$_2$, showing the pH reduction due to CO$_2$ absorption. Figure 2 illustrates the CO$_2$ reduction peaks for various electrolytes. These peaks were obtained using the LSV method to assess the correlation between the IL structure and the potential onset. Consequently, the potential onset followed a specific order beginning with the most positive) (see Table 1). Therefore, this outcome implied that no correlation between pH and onset reduction potential was observed. Meanwhile, Snuffin et al. (2011) explained that the catalytic reduction of CO$_2$ using IL salts was caused by the interaction between CO$_2$ and the anions of ILs, which was based

![Figure 2. CO$_2$ reduction peaks for different 0.1 M 0.1 NaHCO$_3$ on the Lewis acid-base mechanism.](image)

The CO$_2$ER reaction for the selected electrolytes was performed using CA for 2 h. Table 2 lists the applied potentials for the selected electrolytes and their corresponding current density values, as shown in Figure 3. Confirming Ohm’s law, a higher applied potential resulted in higher current density. Moreover, the electrolyte containing the 0.1 M NaHCO$_3$ + 0.02 M EMIM BF$_4$ produced a lower applied potential and higher current density than the solution without IL. This finding was highly favourable for the CO$_2$ER system, in which the significantly higher current density was attributed to the enhanced conductivity arising from a higher concentration of ions in the solution. Therefore, this enhancement provided more charge carriers to facilitate the electric current conduction.

Nevertheless, a substantially lower current density at the same applied potential was observed for the 0.1 M NaHCO$_3$ + 0.02 M BMIM GLY electrolyte than the solution containing EMIM BF$_4$. This outcome could be explained by the strong interaction between glycinate ions and CO$_2$ through chemical absorption and extensive solvation, thus limiting the mobility of the ions and

<table>
<thead>
<tr>
<th>Electrolyte</th>
<th>Applied potential (V)</th>
<th>Current density (mA/cm$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference (0.1 NaHCO$_3$)</td>
<td>-1.42</td>
<td>-2.9</td>
</tr>
<tr>
<td>0.1 NaHCO$_3$ + 0.02M EMIM BF$_4$</td>
<td>-1.36</td>
<td>-3.8</td>
</tr>
<tr>
<td>0.1 NaHCO$_3$ + 0.02M BMIM BF$_4$</td>
<td>-1.48</td>
<td>-4.9</td>
</tr>
<tr>
<td>0.1 NaHCO$_3$ + 0.02M BBT BF$_4$</td>
<td>-1.44</td>
<td>-4.84</td>
</tr>
<tr>
<td>0.1 NaHCO$_3$ + 0.02M BMIM GLY</td>
<td>-1.36</td>
<td>-2.77</td>
</tr>
</tbody>
</table>

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Table 1. The pH values for the selected electrolytes before and after purging CO$_2$. A study by Whipple et al. (2010) highlighted a negative correlation between pH value and concentration of protons (H$^+$) in the solution (lower pH = higher H$^+$), producing a higher CO$_2$ protonation. Given that the hydrogen evolution reaction (HER) rate competing with the CO$_2$ reduction reaction for electrons decreased, the production rates of the desired products were accelerated. On the contrary, this study presented that the sequence of potential onsets (starting from the most positive) (see Table 1). Therefore, this outcome implied that no correlation between pH and onset reduction potential was observed. Meanwhile, Snuffin et al. (2011) explained that the...
decreasing current density (Mohammed et al., 2023). The same explanation could also describe the 0.1 M NaHCO₃ + 0.02 M BMIM GLY electrolyte demonstrating the lowest pH value. Nevertheless, this condition could be avoided by choosing an electrolyte with high basicity.

The alkyl chain length negatively impacted the transport parameters (conductivity and cation diffusion coefficients) (Every et al., 2004). Considering that the length of the alkyl chains in the cation increased, the packing density of the ions dropped, and the space between the cation and anion increased. This process weakened the ion-ion interactions and reduced the dissociation of the ions in the IL, causing a decrease in ionic conductivity. On the contrary, shorter alkyl chains resulted in a greater packing density of the ions and stronger ion-ion interactions, leading to improved ion dissociation and increased ionic conductivity.

3.2 CO₂ ER in 0.1 M NBu₄PF₆ ACN-Based solution

Figure 4 displays the CO₂ reduction peaks for different 0.1 M NBu₄PF₆ ACN-based electrolytes with and without ILs. The CO₂ reduction potential was lower in all electrolytes containing ILs than in the reference electrolyte. The [EMIM][BF₄] electrolyte solution exhibited a lower overpotential of 320 mV compared to the reference solution. Rosen et al. (2011) observed that [EMIM][BF₄] demonstrated a 96% faradaic efficiency on the silver cathode (Ag) and a significant capability to decrease the overpotential (approximately 200 mV higher than the equilibrium potential). Furthermore, the electrostatic interaction reduced when the alkyl chain length increased. This process reduced the transport characteristics, leading to more negative onset potential.

Table 3 summarises the results of the CA study at the applied potential and the corresponding current density value for each electrolyte after running the experiment for 30 minutes, with the corresponding graph in Figure 5. The ILs were observed to improve the current density, even at a lower potential than the reference electrolyte. This outcome was attributed to the higher mobility of IL ions compared to the larger structure of NBu₄PF₆.

![Figure 3: Chronoamperometry results for 0.1 NaHCO₃ aqueous electrolytes with and without ILs](image1)

![Figure 4: CO₂ reduction peaks in different 0.1 M NBu₄PF₆ acetonitrile-based electrolytes with and without ILs](image2)

<table>
<thead>
<tr>
<th>Electrolyte</th>
<th>Applied potential (V)</th>
<th>Current density (mA/cm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference (0.1 M NBu₄PF₆ in ACN)</td>
<td>-2.64</td>
<td>-3.40</td>
</tr>
<tr>
<td>0.1 M NBu₄PF₆ in ACN + 0.02M EMIM BF₄</td>
<td>-2.32</td>
<td>-4.40</td>
</tr>
<tr>
<td>0.1 M NBu₄PF₆ in ACN + 0.02M EMIM TFSI</td>
<td>-2.33</td>
<td>-4.60</td>
</tr>
<tr>
<td>0.1 M NBu₄PF₆ in ACN + 0.02M BMIM BF₄</td>
<td>-2.39</td>
<td>-4.40</td>
</tr>
<tr>
<td>0.1 M NBu₄PF₆ in ACN + 0.02M BBT BF₄</td>
<td>-2.42</td>
<td>-3.32</td>
</tr>
<tr>
<td>0.1 M NBu₄PF₆ in ACN + 0.02M BBT TFSI</td>
<td>-2.44</td>
<td>-3.60</td>
</tr>
<tr>
<td>0.1 M NBu₄PF₆ in ACN + 0.02M HMIM TFSI</td>
<td>-2.34</td>
<td>-4.30</td>
</tr>
</tbody>
</table>
The applied potential for the same current density at 4.4 mA/cm² was also slightly higher for BMIM BF₄ with a longer alkyl chain when comparing the electrolytes containing EMIM BF₄. In addition, the influence of the alkyl chain was more pronounced for BBT BF₄. At a similar applied voltage, the BBT BF₄ exhibited significantly reduced current density compared to BMIM BF₄ due to the presence of the dibutyl chain on the triazolium ring. Thus, this outcome further confirmed that an increase in the alkyl chain length led to decreased ion mobility and increased resistance towards the electrode.

Further investigation of the effects of the IL structure on the molecular orbitals and CO₂ER was performed due to inadequate conclusive evidence. The frontier molecular orbital theory states that the interaction between a Lewis acid and a Lewis base occurs through the interaction of specific frontier orbitals of the acid and base (Fukui, 1975; Liu et al., 2020). This interaction involves the transfer of electrons from the HOMO level of the base to the LUMO level of the acid. Therefore, the impact of molecular orbital levels on CO₂ reduction potential is highly relevant. Figure 6 portrays the HOMO and LUMO values of [EMIM], [BMIM], [BBT], [BF₄], [TFSI], and [GLY] calculated using TmoleX.

A significantly higher HOMO value was observed for the [GLY] anion than the [BF₄] anion. Even though the [GLY] anion also demonstrated a notably lower current density than the [BMIM][BF₄], a more favourable onset potential was presented (see Figure 3). Given that CO₂ was the Lewis acid and anions were the Lewis base, anions with higher HOMO values possessed a more significant positive reduction potential. A study by Gomes et al. (2022) also highlighted that the [TFSI] anion produced a decreased capability for reducing CO₂ compared to [BF₄]. Typically, the [TFSI] anion exhibits a greater HOMO value in comparison to [BF₄]. Therefore, the anions with higher HOMO values improved the efficiency of CO₂ER by reducing the overpotential. Nonetheless, a significant pH decrease was observed for a strong acid or base interaction between the anion and CO₂ (such as glycinate), which produced a detrimental effect on reducing the current density.

Another study by Monteiro et al. (2021) presented three main hypotheses on the impact of cations on the activity and selectivity of electrocatalytic processes at the interface. These hypotheses suggested that the cations modified the local electric field, buffer the interfacial pH, or stabilise reaction intermediates. The study also explained that cation acidity substantially impacted the CO₂ER, which acidic cations promoted CO₂ER at low overpotentials and in acidic media. Meanwhile, Lau et al. (2016) described that the acidic proton at the C₂ position of the...
imidazolium ring stabilised the intermediate CO$_2$ anion radical by forming hydrogen bonds, which rendered it a significant catalytic site. Similarly, Neyrizi et al. (2022) concluded a direct correlation between the performance of CO$_2$ reduction and acidity of the imidazolium cation (C$_2$-H).

This study investigated the cation effect on CO$_2$ ER by examining the CO$_2$ reduction for the same anion. Figure 2 illustrates that for the same anion, the order of CO$_2$ reduction for [BF$_4$] (starting from the more positive onset potential) was [EMIM][BF$_4$] > [BMIM][BF$_4$] > [BBT][BF$_4$]. In contrast, the sequence of cation acidity did not follow a similar trend as the CO$_2$ reduction overpotential, in which the order of LUMO values of the cations (starting from the lowest) was [BBT] < [BMIM] < [EMIM]. Our previous study deduced that a low LUMO value of the cation (acidity) enhanced the solubility of CO$_2$ by facilitating an acid/base interaction between the cation and the negatively charged oxygen (Mohammed et al., 2023). Therefore, a long cation alkyl chain could present difficulties reaching the electrode surface, impeding its proximity with the electrons. This observation was attributed to the positively charged nitrogen atom of the cation that was relatively far from the electrode surface due to the long alkyl chain.

Coulomb’s law states that the electrostatic attraction or repulsion intensity between two-point charges is directly proportional to the product of their magnitudes and inversely proportional to the square of the distance between them. A study by Azra et al. (2022) supported this statement by demonstrating the correlation between long alkyl chains and molecular interaction. The study highlighted the significance of chain length in separating organic and aqueous phases, in which longer chain lengths promoted easy separation. In contrast, shorter chain lengths enhanced water clarity, hindering complete separation and resulting in lower extraction efficiency. Considering that the disparity in the LUMO values between the cations was not substantial, the long alkyl chain of a cation decreased the interaction between its positively charged nitrogen and the electrons on the electrode to a greater extent than the magnitude of the charge. When an electric potential was provided, the positively charged ions migrated towards the negatively charged electrode (cathode). Consequently, the long non-polar alkyl chain decreased or increased the mobility of the ions or resistance towards the electrode, respectively.

Figure 5 demonstrates that the inclusion of ILs significantly improves the system. This observation was due to the inclusion of ILs enhancing the acid or base interaction with CO$_2$. Additionally, a higher non-polar/non-polar interaction with CO$_2$ and lower acid/base interaction was observed owing to the large structure and the long alkyl chain of NBu$_4$PF$_6$. Figure 7 depicts the sigma profile and sigma potential of the cations and anions. Similar to CO$_2$, the NBu$_4$PF$_6$ was highly non-polar. Overall, the CO$_2$ exhibited a dual nature, with both partially charged properties that allowed it to interact with its environment through acid/base interaction and non-polar characteristics (due to the linear structure of its bonds). Thus, the CO$_2$ ER was greatly affected by the interaction between CO$_2$ and the electrolyte environment.

Another study by Ueno et al. (2010) denoted that the solvation of strongly Lewis basic anions and highly Lewis acidic cations by solvents enabled a substantial level of salt dissociation. Therefore, selecting a favourable combination of ILs with a short alkyl chain, an anion with a high HOMO value, and a compatible

![Figure 7](https://www.example.com/figure7.png)

**Figure 7**: Sigma profile (a) and sigma potential (b) of the cations and anions of ILs including CO$_2$.
solvent increased the current density. The performance of the CO₂ER system was also reduced when the non-polar/non-polar interaction between the ILs and CO₂ was dominant. Thus, cations with short alkyl chains and anions with high HOMO values were essential to improve the acid/base interaction between CO₂ and electrolytes for optimal performance of ILs in CO₂ER. Notably, cations with short alkyl chains lowered the resistance to charge resistance at the electrode.

4. Conclusion

In this study, the CO₂ reduction peaks, and the current density of different electrolytes were evaluated using linear sweep voltammetry (LSV), and chronoamperometry (CA). HPLC and GC-TCD were used to confirm the formation of the reaction products. The addition of 1-ethyl-3-methylimidazolium tetrafluoroborate [EMIM][BF₄] to the 0.1 M NBu₄PF₆ acetonitrile solution demonstrates that the reduction’s onset potential significantly decreased by 320 mV. It can be concluded that to have effective ionic liquid as electrolyte for CO₂ER reaction, in order to have low overpotential and high current density, the acid/base interaction with IL and CO₂ is desirable, and for that, ILs with small alkyl chain, low LUMO values of cations and high HOMO values as anions are recommended while considering the suitable organic solvent.

5. Acknowledgement

The Fundamental Research Grant Scheme initiative of the Malaysian Ministry of Higher Education provided funding for this study (MOHE-FRGS/1/2021/TK0/UTP/02/12). Additionally, the authors acknowledge the Chemical Engineering Department, the Centre for Research in Ionic Liquids (CORIL), the Centre for Biofuel and Biochemical Research (CBBR), and Centre for Corrosion Research (CCR) of Universiti Teknologi PETRONAS (UTP) for their technical assistance and resources.

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