

CERTIFICATION OF APPROVAL

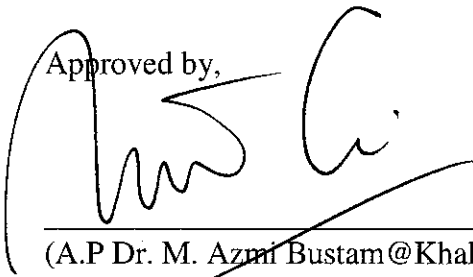
**Carbon Dioxide (CO<sub>2</sub>) Solubility in New Synthesized Ionic Liquid,  
1, 10-bis (trioctylphosphonium-1-yl) decane dioctylsulfosuccinate**

by

Istiazah Ab. Aziz

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Approved by,



(A.P Dr. M. Azmi Bustam @Khalil)

~~A.P. Dr. Mohamed Azmi Bustam @Khalil  
Assoc. Professor  
Chemical Engineering Programme  
Universiti Teknologi PETRONAS~~

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

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## CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

ISTIAZAH AB. AZIZ

## **ACKNOWLEDGEMENT**

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## ABSTRACT

Due to the potential of ionic liquids (ILs) for industrial application in carbon dioxide (CO<sub>2</sub>) capture and gas separation processes, solubility of near or supercritical CO<sub>2</sub> in ionic liquids has been an extensive research during the last few years. This work studies the solubility of CO<sub>2</sub> in phosphonium-based ionic liquids that, unlike imidazolium-based ILs, have received little attention in spite of their interesting characteristics.

This work addresses the study of solubility of CO<sub>2</sub> in phosphonium-based ionic liquid, at temperature (298.15, 303.15 and 308.15) K and pressure ranging from 15-25 bars. Phosphonium-based ionic liquids have attractive characteristics such as negligible vapor pressures, high thermal stability, large liquidus range and nonflammability, high solvation capacity, compatibility with strong alkaline solutes, stabilizing effect on palladium catalysts, effective media for Heck and Suzuki reactions and their low cost. [4]

Removal of CO<sub>2</sub> in natural gas and other gas sources commonly used chemical solvents comprise amine solutions. Commercial amine solutions useable for this purpose include monoethanolamine (MEA), N-methyldiethanolamine (MDEA), and diethanolamine (DEA). Although an effective CO<sub>2</sub> separation process, amine treating presents several issues and challenges. The present invention provides new data of the alternative solvent for CO<sub>2</sub> removal process which is phosphonium-based ionic liquid.

The solubility measurement is using experimental approach. The experimental setup is established and leakage test is run to confirm the setup is really efficient. 2.00 g of the ionic liquid was put in the pressure cell directly from the oven, and immediately the pressure cell is closed and attached to the unit. Valve a, V<sub>a</sub> is closed while valve b, V<sub>b</sub> and valve c, V<sub>c</sub> are opened. The unit was connected to a vacuum pump and the system is evacuated for 30 minutes. CO<sub>2</sub> gas is introduced to the system by opening V<sub>a</sub>. (The equilibrium condition was judged when the pressure was unchanged). The amount of gas introduced is determined using PVT relation by pressure measurement. V<sub>b</sub> is opened

so that ionic liquid sample could be in contact with CO<sub>2</sub> gas. After equilibrium as indicated by negligible pressure change, the pressure is measured again to determine the amount of CO<sub>2</sub> gas left in vapor phase. The different in the amount of CO<sub>2</sub> gas is taken as the amount of CO<sub>2</sub> dissolves.

Solubility of CO<sub>2</sub> gas in ionic liquid is determined based on CO<sub>2</sub> gas molality and the mole fraction between the number of moles of CO<sub>2</sub> gas absorbed in ionic liquid and the number of moles of ionic liquid used in the experiment. The relationship between pressure and mole fraction of CO<sub>2</sub> gas in ionic liquid is analyzed. Henry's constant of CO<sub>2</sub> in this phosphonium-based ionic liquid also was determined and graph of Henry's constant versus inverse temperature is plotted.

Finally, new experimental results for the solubility of CO<sub>2</sub> in the new synthesized ionic liquid [P<sub>888</sub>C<sub>10</sub>P<sub>888</sub>] docusate are presented for temperatures 298.15 K, 303.15 K, and 308.15 K and pressures ranging from 15 to 25 bars. Henry's law constants are determined from that solubility pressure data. The solubility pressures were correlated by means of extended Henry's law.

# TABLE OF CONTENTS

|   |     |
|---|-----|
| <b>CERTIFICATION</b>                      | i   |
| <b>ACKNOWLEDGEMENT</b>                    | ii  |
| <b>ABSTRACT</b>                           | iii |
| <b>CHAPTER 1: INTRODUCTION</b>            |     |
| 1.2 Background of Study                   | 1   |
| 1.2 Problem Statement                     | 2   |
| 1.3 Objectives and Scope of Study         | 4   |
| <b>CHAPTER 2: LITERATURE REVIEW</b>       | 5   |
| <b>CHAPTER 3: METHODOLOGY</b>             |     |
| 3.1 Solubility Measurement                | 9   |
| 3.2 Establishment of Experimental Setup   | 10  |
| 3.3 Research Methodology                  | 18  |
| <b>CHAPTER 4: RESULTS AND DISCUSSIONS</b> |     |
| 4.1 Experimental Setup Leakage Test       | 26  |
| 4.2 Determination of Volume 1, $V_1$      | 28  |
| 4.3 Solubility Measurement                | 32  |
| <b>CONCLUSION</b>                         | 40  |
| <b>REFERENCES</b>                         | 41  |

## LIST OF TABLES

|  |    |
|--|----|
| Table 2.1: Characteristic of Modern Ionic Liquid     | 7  |
| Table 4.1: Solubility Data at Different Temperatures | 32 |
| Table 4.2: Henry's Law Constant vs Temperature Data  | 38 |

## LIST OF FIGURES

|   |    |
|---|----|
| Figure 1.1: Structure of 1, 10-bis (trioctylphosphonium-1-yl) decane dioctylsulfosuccinate                  | 4  |
| Figure 3.7: Schematic Diagram of the Experimental Apparatus   | 10 |
| Figure 3.1: Top-view of Pressure Cell Design  | 12 |
| Figure 3.2: Pressure Cell Cover Design Cell   | 13 |
| Figure 3.3: Stainless Steel Pressure  | 14 |
| Figure 3.4: Inner View of Stainless Steel Pressure Cell   | 15 |
| Figure 3.5: Frame Work the Experimental Setup   | 16 |
| Figure 3.6: Overall Experimental Setup  | 17 |
| Figure 3.8: Volume 1, $V_1$ ( $V_a$ to $V_b$ )  | 19 |
| Figure 3.9: Volume 2, $V_2$ ( $V_a$ to $V_c$ )  | 19 |
| Figure 3.10: Henry's Law and Raoult's Law Graphs  | 24 |
| Figure 4.1: Spectroscopy for Ionic Liquid without $\text{CO}_2$   | 27 |
| Figure 4.2: Spectroscopy for Ionic Liquid contacted with $\text{CO}_2$                                      | 28 |
| Figure 4.3: Graph Pressure vs $\text{CO}_2$ Mol Fraction at $T=298.15$ K                                    | 33 |
| Figure 4.4: Graph Pressure vs $\text{CO}_2$ Gas Molality at $T=298.15$ K                                    | 33 |
| Figure 4.5: Graph Pressure vs $\text{CO}_2$ Mol Fraction at $T=303.15$ K                                    | 34 |
| Figure 4.6: Graph Pressure vs $\text{CO}_2$ Gas Molality at $T=303.15$ K                                    | 34 |
| Figure 4.7: Graph Pressure vs $\text{CO}_2$ Gas Mol Fraction at $T=308.15$ K                                | 35 |
| Figure 4.8: Graph Pressure vs $\text{CO}_2$ Gas Molality at $T=308.15$ K                                    | 35 |
| Figure 4.9: Pressure vs $\text{CO}_2$ Gas Mol Fraction at $T= 298.15$ K, $T=303.15$ K and $T=308.15$ K      | 36 |
| Figure 4.10: Pressure vs $\text{CO}_2$ Gas Molality at $T=298.15$ K, $T=303.15$ K and $T=308.15$ K          | 36 |
| Figure 4.11: Comparison with Literature Data for Pressure vs $\text{CO}_2$ Gas Mol Fraction at $T=298.15$ K | 37 |
| Figure 4.12: Henry's Law Constant vs Temperature  | 39 |
| Figure 4.13: The Logarithms of the Henry's Law Constant vs Inverse  | 39 |



Temperature

Figure 4.14: Comparison with Literature Data for Logarithms of the Henry's Law Constant vs Inverse Temperature

40

# CHAPTER 1

## INTRODUCTION

### 1.1 BACKGROUND OF STUDY

Recently, ionic liquids (ILs) have attracted much attention due to their unique properties; for example, they have an extremely low vapor pressure, are nonflammable, have excellent solvent power for organic and inorganic compounds, and are easily modified structurally to elicit desired physical properties. Moreover their insignificant vapour pressures, reduces environmental pollution and highly reduces working exposure hazards in comparison with the conventional organic solvents currently being used in the industry.

In the purpose of enhancing sour gases solubility and ultimately replace the hazard volatile organic compounds (VOCs), many researchers have wisely adapted ionic liquids (ILs) to accomplish such task. With the exception of this last type of ILs, where chemical interactions dominate the sorption mechanism, in most ionic liquids the gas solubility is simply driven by a physical absorption mechanism. Among the ILs previously reported in the literature the imidazolium-based ionic liquids, especially those with fluorinated anions such as the bis(trifluoromethylsulfonyl)imide,  $\text{NTf}_2$ , and bis(pentafluoroethyl)trifluorophosphate, pFAP, are the ones with the highest  $\text{CO}_2$  solubilities reported [1,2,3].

In spite of their attractive characteristics, such as negligible vapor pressures, high thermal stability, large liquidus range and nonflammability, high solvation capacity, compatibility with strong alkaline solutes, stabilizing effect on palladium catalysts, effective media for Heck and Suzuki reactions and their low cost [4], the phosphonium-based ionic liquids have received surprisingly little attention in the last few years [5, 6,7]. Some authors have focused their study on the solubility of alcohols [8], alkanes and alkenes [9,10], or even on methane [11], carbon monoxide [12] or oxygen [11] in

phosphonium ILs but few have reported solubilities of carbon dioxide in these ILs [5,9,13].

Ferguson and Scovazzo [14] have shown that imidazolium and phosphonium-based ILs have similar solubilities for several gases. Their study stated that gas solubility of the phosphonium-based ionic liquids is of the same magnitude as the gas solubility for the most familiar imidazolium-based ionic liquids. Henry's law constants in both the imidazolium- and phosphonium-based ionic liquids are similar for carbon dioxide (CO<sub>2</sub>) solubility. In imidazolium-based room temperature ionic liquids (RTILs), the solubility increases as the number of solute carbons increases and when the number of carbon double bonds increases for the hydrocarbon solutes with the same number of carbons. This trend is also observed in phosphonium-based RTILs [14].

Anthony and coworkers [15] suggested that the nature of the anion has the most significant influence on the gas solubility. Hutchings et al. [16] have reported that, at subcritical temperatures, several phosphonium ionic liquids would completely dissolve as soon as all the CO<sub>2</sub> condensed and that the isopleths for these systems follow the vapor pressure curve of the pure CO<sub>2</sub>.

## 1.2 PROBLEM STATEMENT

In the recent past, the amount of experimental and theoretical work on ionic liquids has increased considerably. However, for phosphonium-based ionic liquid there are less well documented academic papers. Phosphonium-based ionic liquids are more thermally stable than imidazolium-based ionic liquids and less expensive to manufacture [17]. So, phosphonium-based ionic liquids are potential to be used to absorb CO<sub>2</sub> instead of using imidazolium-based ionic liquids in the future.

To my knowledge, there is no reported work on the solubility of CO<sub>2</sub> in 1, 10-bis (trioctylphosphonium-1-yl) decane dioctylsulfosuccinate phosphonium-based ionic liquid. Therefore, new solubility data of this phosphonium-based is really important

because solubility is fundamental to most areas of chemistry. Solubility is also one of the most basic of thermodynamic properties. It underlies most industrial processes such as removal of CO<sub>2</sub> in natural gas and other gas sources.

The removal of CO<sub>2</sub> is often required to improve the fuel quality (heating value) of the natural gas. Also, CO<sub>2</sub> in the presence of water can be a corrosive agent to metal pipes. As a consequence, the removal of CO<sub>2</sub> to acceptable specifications is required prior to transport of natural gas or in pipeline. In the natural gas processing industry, various technologies have been employed for CO<sub>2</sub> removal including chemical solvents, physical solvents, and membranes.

By far, chemical solvents that reversibly react with CO<sub>2</sub> are most commonly used for CO<sub>2</sub> removal. Commonly used chemical solvents comprise amine solutions. Commercial amine solutions useable for this purpose include monoethanolamine (MEA), N-methyldiethanolamine (MDEA), and diethanolamine (DEA). In this process, the amine solution (amine and water) circulates in a loop between two key steps: absorption of CO<sub>2</sub> and regeneration of solvent.

Although an effective CO<sub>2</sub> separation process, amine treating presents several issues and challenges as stated below [18]:

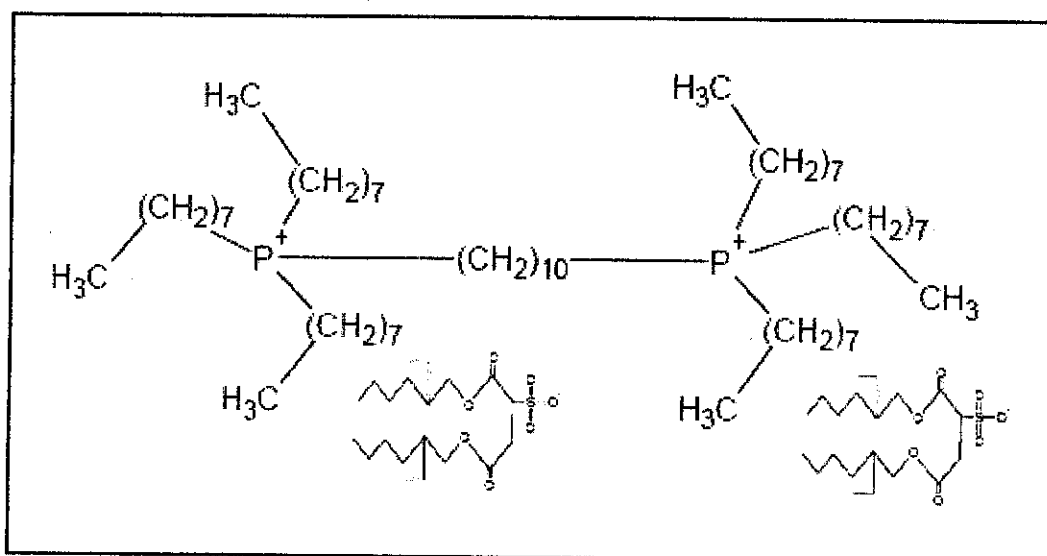
1. Intensive energy required during the regeneration step to break the chemical bonds between the absorbed CO<sub>2</sub> and solvent. Energy is also required to generate steam within the amine regenerator to strip the CO<sub>2</sub> from the solvent.
2. Corrosivity of the amine. Amines can rapidly corrode low alloy steel such as carbon steel.
3. CO<sub>2</sub> loading capacity is limited by concentration (or dilution) of the amine solution.
4. Degradation of amine. Amines react with CO<sub>2</sub> (and H<sub>2</sub>S, COS, etc) to form various different products that are not reversible in the regeneration step. Amine also degrades thermally.

The limitations of the physical and chemical processes discussed above it would be desirable to have a CO<sub>2</sub> removal process with other chemical solvent that require low

energy for regeneration, low solvent losses, minimal corrosion problems, high loading capacity, and thermally stable. The present invention provides new data of the alternative solvent for CO<sub>2</sub> removal process which is phosphonium-based ionic liquid.

### 1.3 OBJECTIVE AND SCOPE OF STUDY

The objective of this study is to measure the solubility of CO<sub>2</sub> gas in new synthesized ionic liquid known as 1, 10-bis (trioctylphosphonium-1-yl) decane dioctylsulfosuccinate [ $P_{888}C_{10}P_{888}$ ] docusate. Molecular formula for this ionic liquid is  $[(C_8H_{17})_3P^+-(CH_2)_{10}-P^+(C_8H_{17})_3] 2Cl^-$ .



**Figure 1.1: Structure of 1, 10-bis (trioctylphosphonium-1-yl) decane dioctylsulfosuccinate**

The new experimental data for the solubility of CO<sub>2</sub> gas in 1, 10-bis (trioctylphosphonium-1-yl) decane dioctylsulfosuccinate phosphonium is taken at temperature (298.15 to 308.15) K and pressures ranging from (15 to 25) bar. Henry's constant of CO<sub>2</sub> in [ $P_{888}C_{10}P_{888}$ ] docusate is determined. The solubility of CO<sub>2</sub> gas in [ $P_{888}C_{10}P_{888}$ ] docusate is determined based on the mole fraction between the number of moles of CO<sub>2</sub> gas absorbed in [ $P_{888}C_{10}P_{888}$ ] docusate and the number of moles of [ $P_{888}C_{10}P_{888}$ ] docusate used in this experiment and also the CO<sub>2</sub> molality.

## CHAPTER 2

### LITERATURE REVIEW

#### 2.1 IONIC LIQUID

Room Temperature Ionic Liquids (RTILs) possess a unique array of physico-chemical properties that make them suitable in numerous task-specific applications in which conventional solvents are non-applicable or insufficiently effective. Such properties include [19]:

- **High thermal stability,**
- **High electrical conductivity,**
- **Large electrochemical window,**
- **Low nucleophilicity and capability of providing weakly coordinating or non-coordinating environment,**
- **Very good solvents properties for a wide variety of organic, inorganic and organometallic compounds: in some cases, the solubility of certain solutes in RTILs can be several orders of magnitude higher than that in traditional solvents.**

In most of these applications, the stability of ionic liquids, at least at a certain extent, is crucial for optimum process performance. Several studies have indicated that, although not 100% inert, certain ionic liquids incorporating 1,3-dialkyl imidazolium cations are generally more resistant than traditional solvents under certain harsh process conditions, such as those occurring in oxidation, photolysis and radiation processes [19].

##### 2.1.1 Color

High quality ionic liquids incorporating [bmim]<sup>+</sup> cation and a variety of anions, such as [PF<sub>6</sub>]<sup>-</sup>, [BF<sub>4</sub>]<sup>-</sup>, [CF<sub>3</sub>SO<sub>3</sub>]<sup>-</sup>, [CF<sub>3</sub>CO<sub>2</sub>]<sup>-</sup> and [(CF<sub>3</sub>SO<sub>2</sub>)<sub>2</sub>N]<sup>-</sup> have been reported to be colorless, even though they are not 100% pure. The color of less pure ionic liquids generally ranges from yellowish to orange. The formation of the color has been

attributed to the use of raw materials with color or excessive heating during the synthesis of imidazolium salt. A number of precautions for synthesis of colorless ionic liquids have been described, and a procedure for removal of color from impure ionic liquids using acidic alumina and activated charcoal has also been proposed [19].

### 2.1.2 Hygroscopicity

The water content has an influence on the viscosity of the ionic liquids. Viscosity measurement indicates that ionic liquids became less viscous with increasing water content. Hydrolysis problems can also occur. [19]

### 2.1.3 Hydrophobicity

The degree of polarity can be varied by adapting the length of the 1-alkyl chain (in 1,3-substituted imidazolium cations), and the counterion. Long-chain IL salts have attracted some interest due to their liquid-crystalline (LC) properties. The anion chemistry has a large influence on the properties of IL. Though little variation in properties might be expected between same-cation salts of these species, the actual differences can be dramatic: for example, [bmim]PF<sub>6</sub><sup>-</sup> is immiscible with water, whereas [bmim]BF<sub>4</sub><sup>-</sup> is water-soluble [19].

The recent interest surrounding ILs in regards to **Green Chemistry** and the associated development of new solvents and alternative technologies has largely been a result of their negligible vapour pressure which inhibits evaporation into the air and allows simple recycling and reuse. The missing vapour pressure has very important advantages compared to other volatile organic chemicals (VOCs). Therefore ionic liquids are not flammable and not explosive and a long range distribution via air can not be expected [19].

|                         |   |
|-------------------------|---|
| A salt                  | Cation or anion quite large                         |
| Freezing Point          | Preferably below 100 <sup>0</sup> C                 |
| Liquidus Range          | Often > 200 <sup>0</sup> C                          |
| Thermal Stability       | Usually High  |
| Viscosity               | Normally < 100cp, workable                          |
| Dielectric Constant     | Implied <= 30                                       |
| Polarity                | Moderate  |
| Specific Conductivity   | Usually < 10 mScm <sup>-1</sup> , “Good”            |
| Molar Conductivity      | < 10 Scm <sup>2</sup> mol <sup>-1</sup>             |
| Electrochemical window  | < 2V, even 4.5 V, except for Bronsted acidic system |
| Solvent and/or catalyst | Excellent for many organic reactions                |
| Vapor pressure          | Usually negligible                                  |

**Table 2.1: Characteristic of Modern Ionic Liquid [20]**

## 2.2 CO<sub>2</sub> SOLUBILITY IN PHOSPHONIUM-BASED IONIC LIQUIDS

There are few studies about solubility of CO<sub>2</sub> in phosphonium-based ionic liquids. Suojiang Zhang *et al.* has studied the solubility of CO<sub>2</sub> in two sulfonate ionic liquids with have phosphonium cations [21]. The study mainly focuses on how difference in anions can contribute to the solubility of CO<sub>2</sub>. The anions that have been used are dodecylbenzenesulfonates and mesylate.

In this paper, the solubility data of CO<sub>2</sub> in sulfonate ionic liquids, such as trihexyl (tetradecyl) phosphonium dodecylbenzenesulfonates ([P<sub>6,6,6,14</sub>][C<sub>12</sub>H<sub>25</sub>PhSO<sub>3</sub>]) and trihexyl (tetradecyl) phosphonium mesylate ([P<sub>6,6,6,14</sub>][MeSO<sub>3</sub>]), at temperatures ranging from (305 to 325) K and pressures ranging from (4 to 9) MPa were presented. The effects of temperature and pressure on the solubility of CO<sub>2</sub> were discussed. The measured data were correlated by the extended Henry's law. The thermodynamic properties of IL–CO<sub>2</sub> systems, such as the standard enthalpy, standard Gibbs free energy, and standard entropy, were obtained [21].



The results from this study shown the Henry's law constants at different temperature presented. It can be seen that the Henry's law constant of all the studied systems increases with increasing temperature, which indicates the solubility of CO<sub>2</sub> decreases with increasing temperature. At a given temperature, the magnitude of the Henry's law constants of CO<sub>2</sub> dissolved in ILs follows the sequence [P<sub>6,6,6,14</sub>][C<sub>12</sub>H<sub>25</sub>PhSO<sub>3</sub>] > [P<sub>6,6,6,14</sub>][MeSO<sub>3</sub>] [21].

## **2.3 COMPARISON BETWEEN PHOSPHONIUM-BASED AND IMIDAZOLIUM-BASED IONIC LIQUIDS**

### **2.3.1 Thermal Stability**

Phosphonium-based ionic liquids are found to be thermally more stable than imidazolium-based ionic liquids [22]. While the thermal decomposition point of neat ionic liquids varies depending on the anion, thermogravimetric analysis (TGA) indicated dynamic thermal stability in excess of 300°C for phosphonium-based ionic liquids [22] and 250°C for most imidazolium-based ionic liquids [23]. The TGA data reported are often not fully indicative since it shows only a dynamic property of the ionic liquid where the ionic liquid is heated for short period of time. Hence, to find the thermal stability of the phosphonium-based ionic liquids, they were analyzed after heating at a temperature of 350°C for over a week [24].

The phosphonium-based ionic liquids were then analysed by GC-MS and they were found to be stable with no decomposition products such as hexane and tetradecyl(dihexyl)phosphine. On the other hand, heating the imidazolium-based ionic liquid 1-butyl-3-methylimidazolium chloride at 250°C for 1 week resulted in its decomposition as determined by GC-MS analysis [24].

## **CHAPTER 3**

### **METHODOLOGY**

#### **3.1 SOLUBILITY MEASUREMENT**

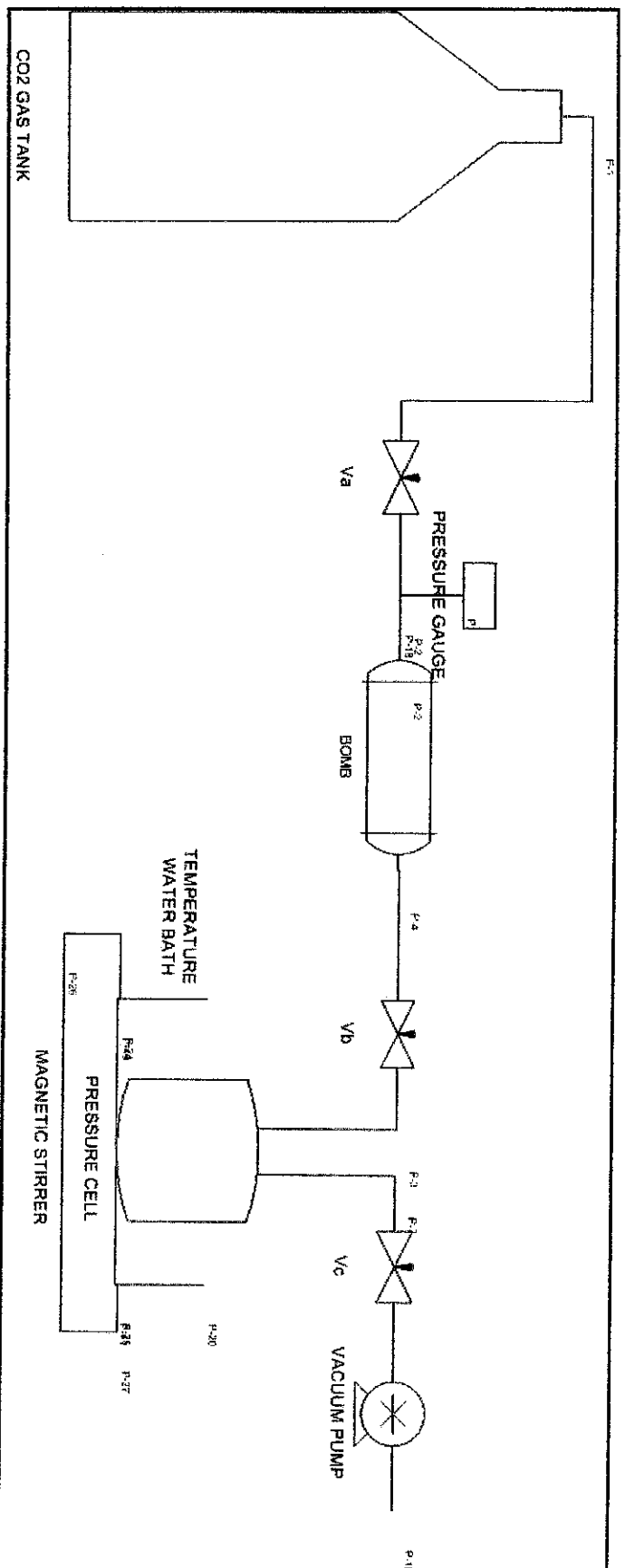
##### **3.1.1 Introduction to Solubility Measurement**

Solubility is measured in terms of mol of CO<sub>2</sub> gas absorbed into the ionic liquid to the mol of ionic liquid used in this experiment. The mole of CO<sub>2</sub> can be calculated using Ideal Gas Law.

##### **3.1.2 Solubility Measurement Experimental Setup**

The apparatus used for CO<sub>2</sub> solubility measurement consists of a stainless steel pressure cell, a CO<sub>2</sub> gas storage tank, a bomb, a pressure gauge, a vacuum pump, valves, a magnetic stirrer and a temperature water bath; a schematic diagram of the experimental setup is shown in Figure 3.1.

### 3.2 ESTABLISHMENT OF THE EXPERIMENTAL SETUP



**Figure 3.1: Schematic Diagram of the Overall Experimental Setup**

The system is designed so that CO<sub>2</sub> solubility measurement could be repeated several times with the same ionic liquid sample.

### 3.2.1 Pressure Cell

Pressure cell is designed as the container for  $[P_{388}C_{10}P_{388}]$  docusate. The volume of the pressure cell is calculated as below:

$$\text{Volume, } V = \pi(D/2)^2 h$$

Where

Diameter,  $D = 4.0\text{cm}$

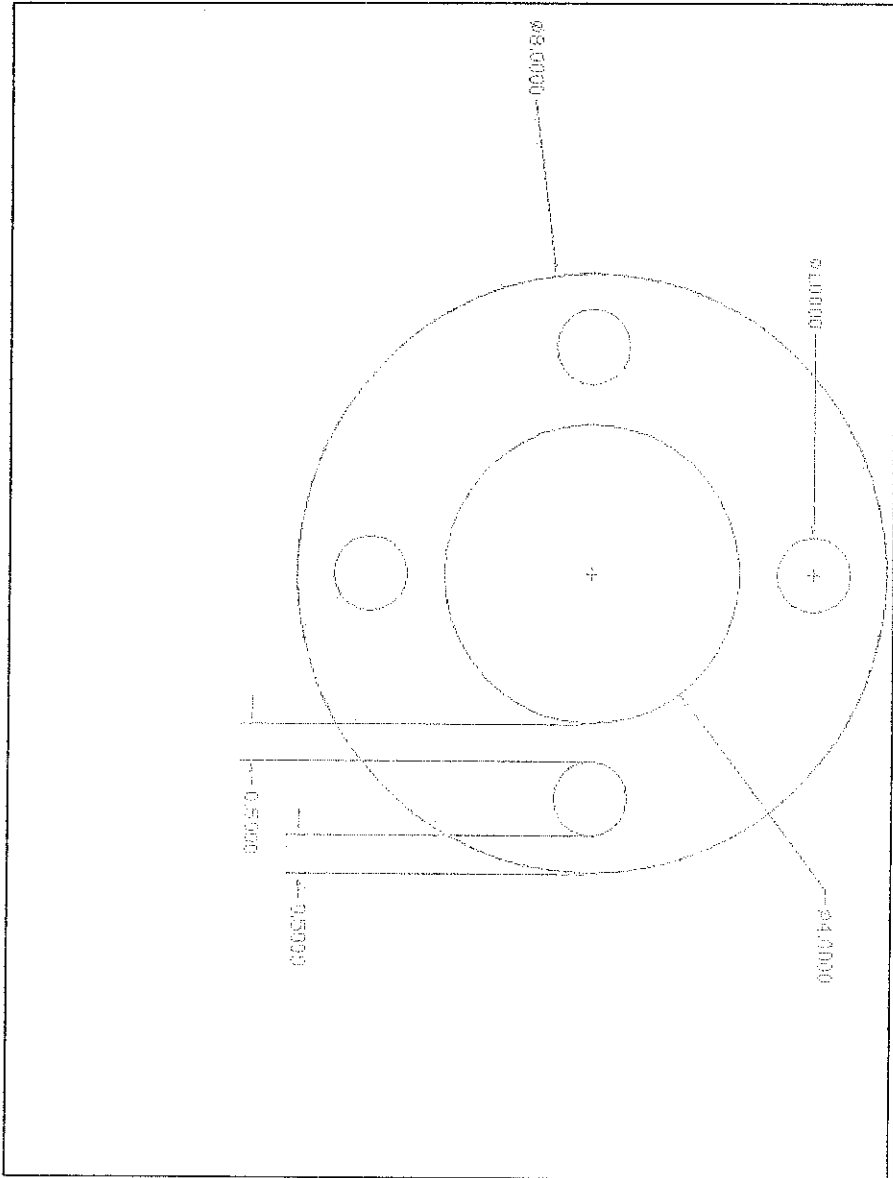
Height,  $h = 1.0\text{cm}$

$$\begin{aligned}\text{Calculated Volume will be} &= \pi(4/2)^2 \times 1 \\ &= 12.5664 \text{ cm}^3\end{aligned}$$

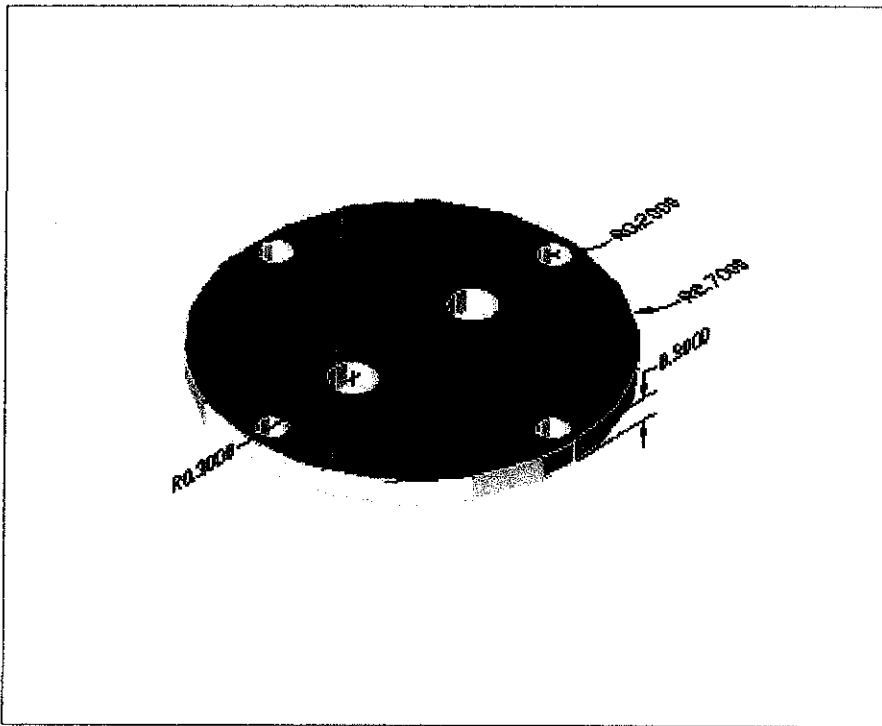
The pressure cell will attaches to:

- Valve b,  $V_b$
- Release Valve,  $V_c$

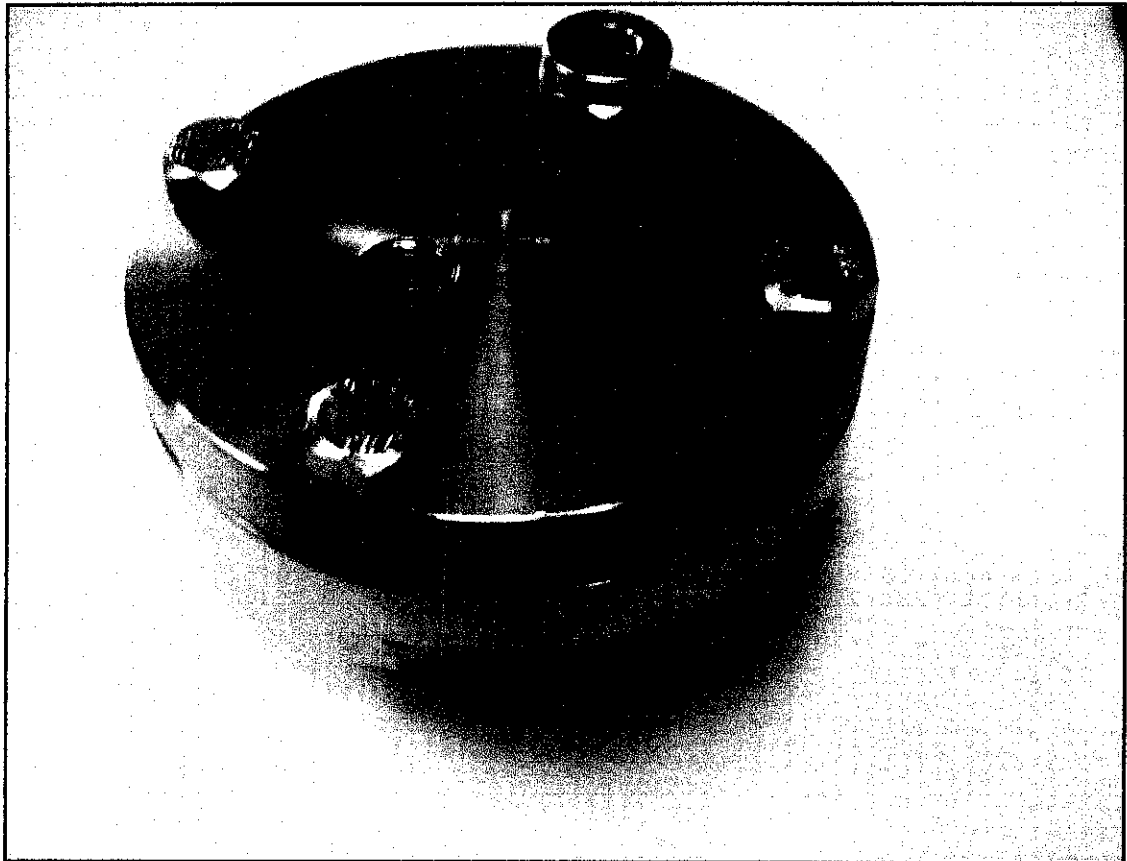
The o-ring will be used between the cover and the pressure cell it self in order to prevent any leakage occurs. Figure 3.1 to 3.2 shows the design of pressure cell and its covers. Figure 3.3 shows the pressure cell that had been fabricated.



**Figure 3.2: Top-view of Pressure Cell Design**



**Figure 3.3: Pressure Cell Cover Design**



**Figure 3.4: Outer View of Stainless Steel Pressure Cell**

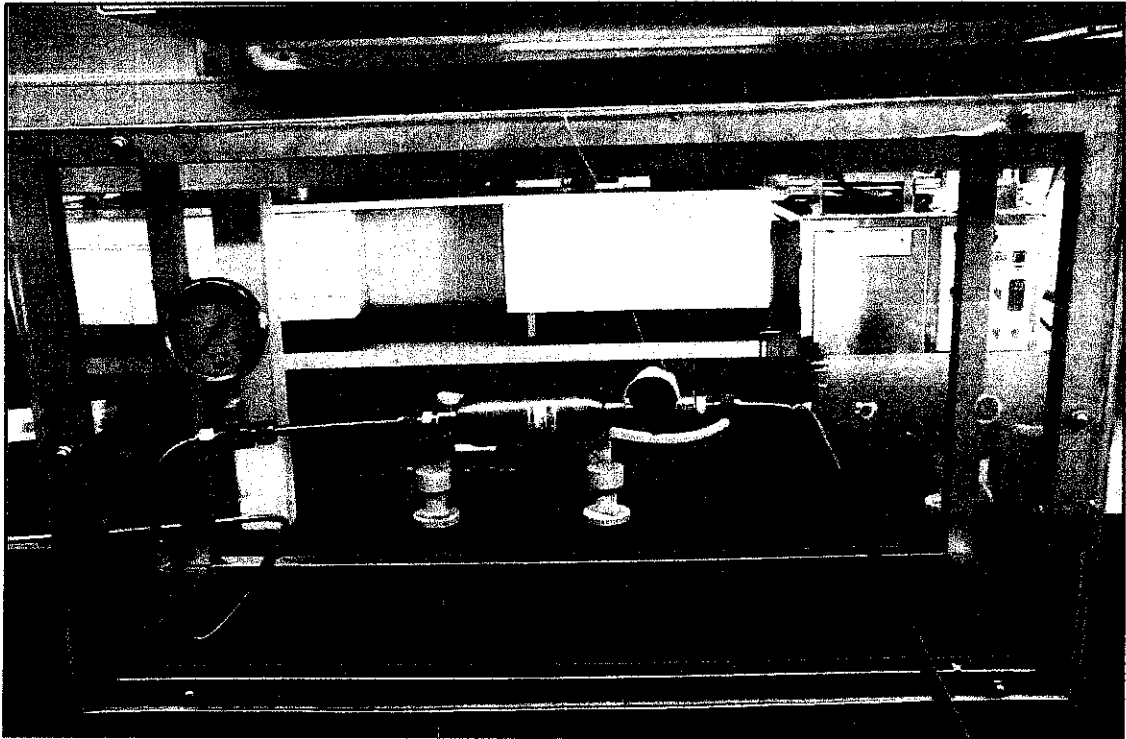


**Figure 3.5: Inner View of Stainless Steel Pressure Cell**



### 3.2.2 Frame Work

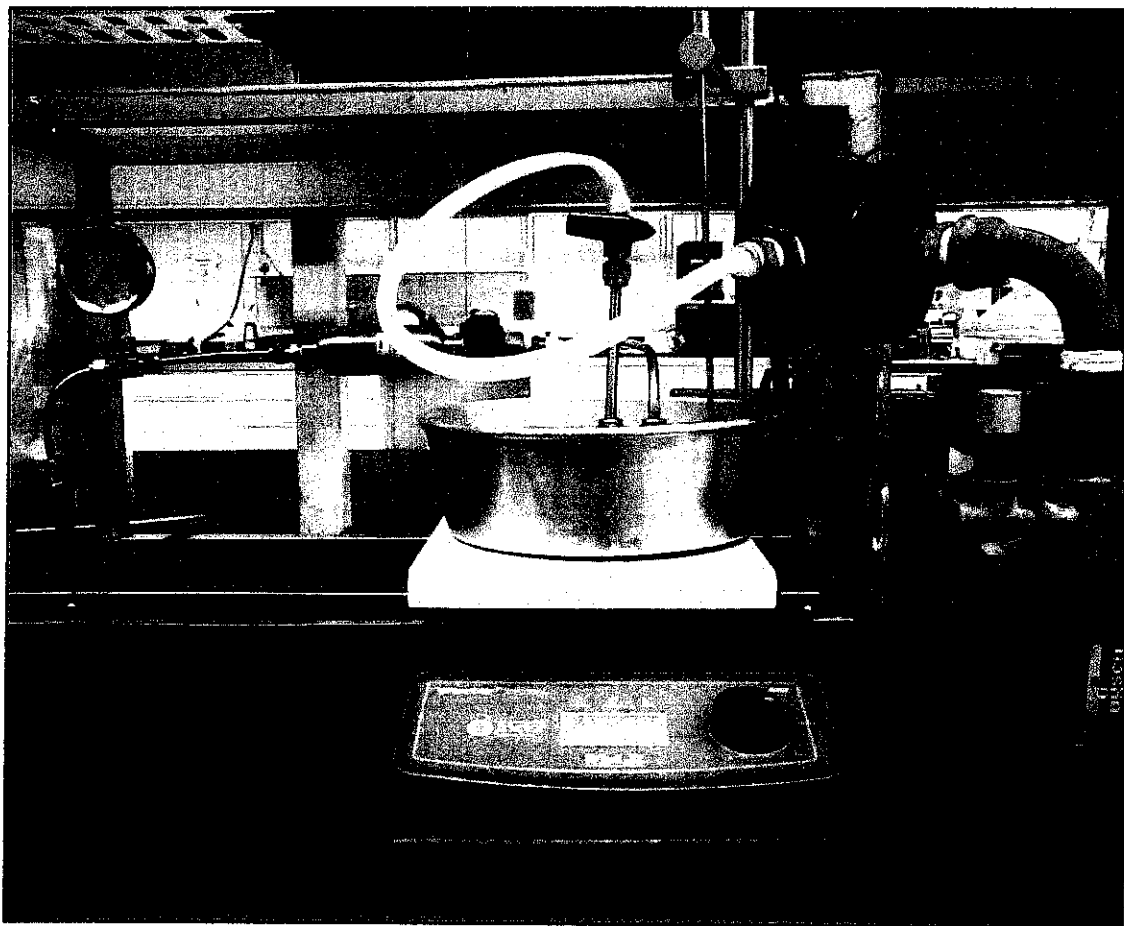
The frame work has been constructed to attach the experimental apparatus such as valves, and pressure gauge. Below is the design of the frame work.



**Figure 3.6: Frame Work for the Experimental Setup**

### 3.2.3 Overall Experimental Setup

The pressure cell that has been designed is attached to the frame work. Vacuum pump and CO<sub>2</sub> tank also are connected to the setup. Below is the overall experimental setup for CO<sub>2</sub> solubility measurement.



**Figure 3.7: Overall Experimental Setup**

### **3.3 RESEARCH METHODOLOGY**

#### **3.3.2 Spectroscopy Test**

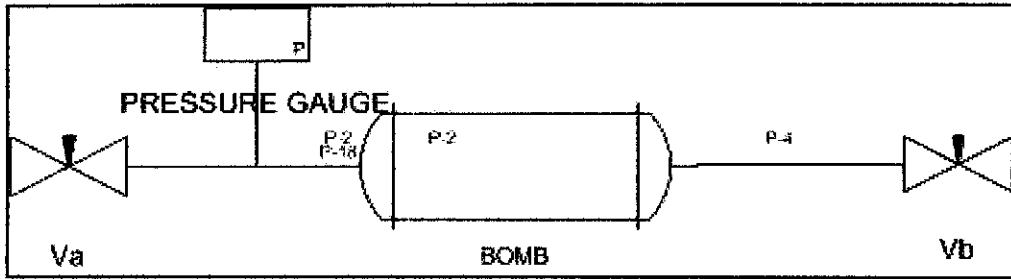
1. FTIR spectrum is taken before and after the CO<sub>2</sub> is introduced to the ionic liquid.
2. For the ionic liquid without CO<sub>2</sub>, the sample is dried in vacuum oven and directly put into the Shimadzu model IR Spectrometer.
3. For the ionic liquid contacted with CO<sub>2</sub>, it is collected after the solubility measurement is finished.
4. The broadband trend of the ionic liquid with and without CO<sub>2</sub> contact is evaluated.

#### **3.3.3 Procedure of Experimental Setup Leakage Test**

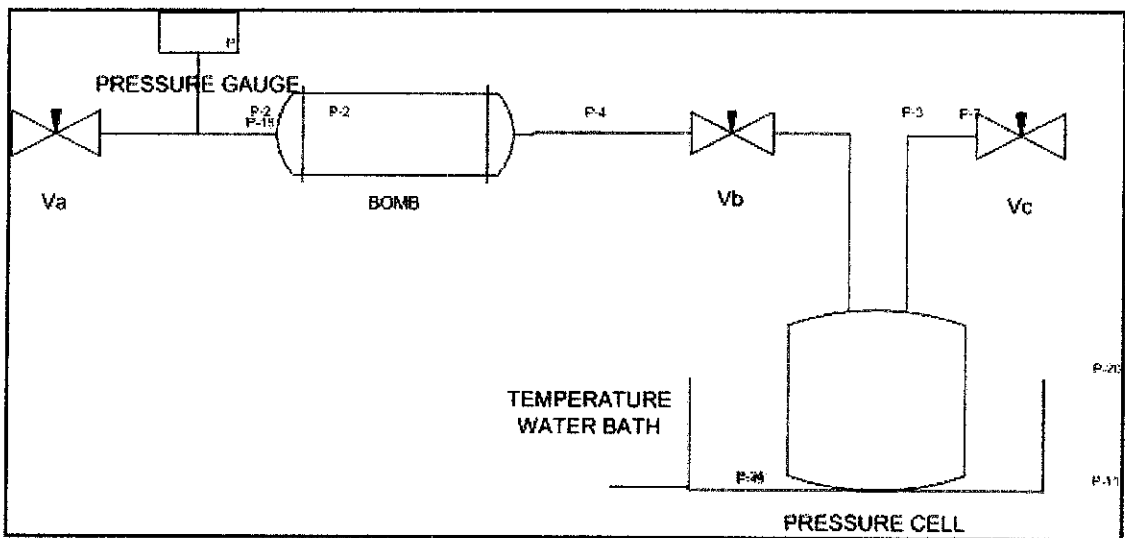
1. Vacuum is applied to the whole system to ensure no other gases in the system.
2. 255 psi CO<sub>2</sub> gas is introduced to the first line of the system by opening valve a, V<sub>a</sub> while valve b, V<sub>b</sub> and valve c, V<sub>c</sub> is closed.
3. The pressure reading showed by pressure gauge is monitored for 5-8 hours.
4. V<sub>b</sub> is opened to let the CO<sub>2</sub> gas exposed to the whole system. V<sub>c</sub> is maintain closed all the time.
5. The pressure reading showed by pressure gauge is monitored for 24 hours.

### 3.3.4 Procedure of Volume, $V_1$ Determination

Figure 3.8 and 3.9 show initial volume and volume 1,  $V_1$ .



**Figure 3.8: Initial Volume,  $V_{\text{initial}}$  ( $V_a$  to  $V_b$ )**



**Figure 3.9: Volume 1,  $V_1$  ( $V_a$  to  $V_c$ )**

1. Vacuum is applied to the whole system to ensure no other gases in the system.
2. 250 psi  $\text{CO}_2$  gas is introduced to the system as  $P_1$
3.  $V_a$  and  $V_b$  is closed
4.  $V_c$  is opened to release the left  $\text{CO}_2$  gas
5. The pressure reading is observed till it stable
6.  $V_b$  is opened
7. The pressure reading is taken as  $P_2$
8.  $V_1$  is determined by using formula  $P_{\text{initial}} V_{\text{initial}} = P_1 V_1$

### 3.3.5 Procedure of Solubility Measurement

1. Ionic liquid is dried for 24 hours at 80°C in the vacuum oven.
2. 2.00 g of the ionic liquid was put in the pressure cell directly from the oven, and immediately the pressure cell is closed and attached to the unit.
3. Valve a,  $V_a$  is closed while valve b,  $V_b$  and valve c,  $V_c$  are opened.
4. The unit was connected to a vacuum pump and the system is evacuated for 30 minutes.
5. The vacuum pump is switch off.
6.  $V_c$  and  $V_b$  are closed.
7. The temperature of the hot plate stirrer is adjusted to be 25 °C.
8. CO<sub>2</sub> gas is introduced to the system by opening  $V_a$ . (The equilibrium condition was judged when the pressure was unchanged). The amount of gas introduced is determined using PVT relation by pressure measurement.
9.  $V_b$  is opened so that ionic liquid sample could be in contact with CO<sub>2</sub> gas.
10. After equilibrium as indicated by negligible pressure change, the pressure is measured again to determine the amount of CO<sub>2</sub> gas left in vapor phase. The different in the amount of CO<sub>2</sub> gas is taken as the amount of CO<sub>2</sub> dissolves.
11. Valve  $V_c$  is kept closed throughout series of run.
12. Pressures are measured before opening valve  $V_b$  and after equilibration with valve  $V_b$  is opened.
13. The procedure is repeated for measurement at different pressures.
14. The mol of ionic liquid,  $n_i$  is calculated based of pure ionic liquid used in this solubility measurement.

### 3.3.6 Data Interpretations

#### 3.2.6.1 Mole Fraction of CO<sub>2</sub> gas in [P<sub>888</sub>C<sub>10</sub>P<sub>888</sub>] docusate

The amount of CO<sub>2</sub> gas is determined by the Ideal Gas Law. It is a good approximation to the behavior of many gases under many conditions. The equation as below:

$$PV = nRT$$

Where

**P** is the absolute pressure of the gas (Pa)

**Absolute Pressure = Gauge Pressure + Atmospheric Pressure**

**V** is the volume of the gas (m<sup>3</sup>)

**n** is the amount of substance of the CO<sub>2</sub> gas (mol)

**R** is the gas constant (8.3144 JK<sup>-1</sup>mol<sup>-1</sup>)

**T** is the absolute temperature (K)

**The Kelvin scale is called absolute temperature**

The volume of CO<sub>2</sub> gas introduced into the system is volume 1, V<sub>1</sub>.

$$P_1 V_1 = P_{\text{initial}} V_{\text{initial}}$$

The number of moles of CO<sub>2</sub> gas introduced into the system, n<sub>1</sub> is calculated using Ideal gas Law.

$$n_1 = P_1 V_1 / RT$$

The number of moles of CO<sub>2</sub> gas that is absorbed into [P<sub>888</sub>C<sub>10</sub>P<sub>888</sub>] docusate, n<sub>absorb</sub> is calculated using the equations below. (V<sub>1</sub> and V<sub>2</sub> are assumed to be the same)

$$P_1 V_1 / n_1 = P_2 V_2 / n_2$$

$$n_{\text{absorb}} = n_2 - n_1$$

The number of moles of  $[P_{888}C_{10}P_{888}]$  docusate used in this experiment,  $n_i$  is calculated using the equation below.

$$n_i = m_i / M_i$$

$$n_i = (2.0 \text{ g}) / (1624 \text{ g/mol})$$

$$n_i = 0.001231527 \text{ mol}$$

The mole fraction of  $CO_2$  gas absorbed to  $[P_{888}C_{10}P_{888}]$  docusate,  $X_{CO_2(\text{absorb})}$  is ratio between the number of mole of  $CO_2$  gas absorbed in  $[P_{888}C_{10}P_{888}]$  docusate to the number of moles of  $CO_2$  absorbed,  $n_{\text{absorb}}$  and number of moles of  $[P_{888}C_{10}P_{888}]$  docusate,  $n_i$  used in this experiment.

$$X_{CO_2(\text{absorb})} = n_{\text{absorb}} / (n_{\text{absorb}} + n_i) \quad [30]$$

$CO_2$  gas molality,  $m_{CO_2}$  is the amount of substance (the number of moles) of  $CO_2$  per kilogram of  $[P_{888}C_{10}P_{888}]$  docusate.

$$m_{CO_2} = n_{\text{absorb}} / 0.002 \text{ kg}$$

Where

$n_1$  is amount of  $CO_2$  gas introduced into the system (mol)

$n_2$  is amount of  $CO_2$  gas after equilibrium condition is achieved (mol)

$n_{\text{absorb}}$  is amount of  $CO_2$  absorbed by the ionic liquid (mol)

$X_{CO_2(\text{absorb})}$  is the mol fraction of  $CO_2$  in ionic liquid (dimensionless)

$n_i$  is the amount of ionic liquid (mol)

$m_{CO_2}$  is the mass of ionic liquid (mol/kg)

$M_i$  is the molar mass of ionic liquid (g/mol)

$P_1$  is pressure when the  $CO_2$  gas is introduced into the system (Pa)

$P_2$  is pressure after the equilibrium condition is achieved (Pa)

$V_1$  is volume of CO<sub>2</sub> gas introduced into the system (m<sup>3</sup>)

$V_2$  is volume of CO<sub>2</sub> gas after the equilibrium condition is achieved (m<sup>3</sup>)

$V_p$  is volume of pressure cell (m<sup>3</sup>)

$V_i$  is volume of ionic liquid (m<sup>3</sup>)

$T$  is Temperature (K)

$R$  is 8.314472 JK<sup>-1</sup>mol<sup>-1</sup>

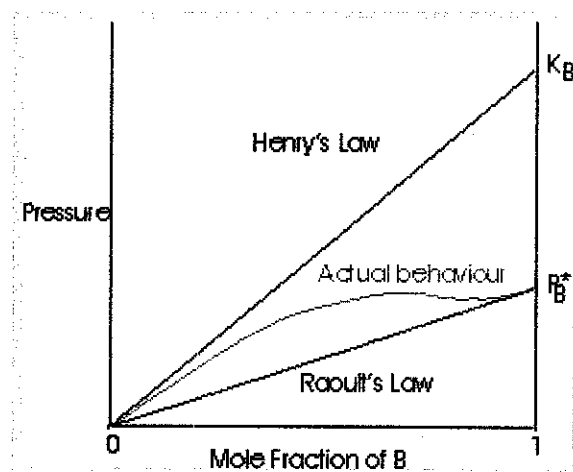
### 3.2.6.2 Henry's Law Constant

In an ideal solution of two liquids, both components obey Raoult's Law. However, it has been experimentally observed that, for real solutions at low concentrations, although the solvent (the major component of the solution) usually obeys Raoult's Law, the solute (the minor component of the solution) does not. The vapour pressure of the solute is proportional to its mole fraction, but the constant of proportionality is not the vapour pressure of the pure substance. This relationship is defined in Henry's Law:

$$p_B = x_B K_B$$

Note the solute is labeled as substance B to avoid confusion with the solvent, labeled A.  $x_B$  is the mole fraction of the solute, and  $K_B$  is an empirically determined constant with the dimensions of pressure, chosen so that on a graph of the vapour pressure of B against its mole fraction, the Law gives a tangent to the experimental curve at  $x_B = 0$  :





**Figure 3.10: Henry's Law and Raoult's Law Graphs**

Mixtures for which the solute obeys Henry's Law and the solvent obeys Raoult's Law are called ideal-dilute solutions. Note  $K_B$  may be greater or less than  $p_B^*$ .

The reason that the behaviours of solvent and solute differ so markedly at low concentrations is intuitively quite obvious. The solvent is in large excess, so solvent molecules are likely to be surrounded by other solvent molecules. Their environment is very much like that of the pure liquid, and consequently the behaviour of the solvent is very like that of the pure liquid. The solute, on the other hand, is in low concentration, so solute molecules are likely to be surrounded by solvent molecules. Thus their environment is quite different from in the pure solute, and consequently their behaviour is greatly modified.

Exceptions arise when the solvent and solute are of very similar structure. In this instance, though the solute molecules are still surrounded by solvent molecules, their environment is not dissimilar to that in pure solute, their behaviour will not be greatly altered, and both components of the mixture will tend to obey Raoult's Law. This also explains why the greatest deviations from ideality are observed for strongly dissimilar liquids.

In chemistry, Henry's law is one of the gas laws, formulated by William Henry in 1803. It states that at a constant temperature, the amount of a given gas dissolved in a given type and volume of liquid is directly proportional to the partial pressure of that gas in equilibrium with that liquid.

An equivalent way of stating the law is that the solubility of a gas in a liquid at a particular temperature is proportional to the pressure of that gas above the liquid. Henry's law has since been shown to apply for a wide range of dilute solutions, not merely those of gases. Henry's law can be put into mathematical terms (at constant temperature) as shown below:

$$p = K_H c$$

Where  $p$  is the partial pressure of the solute in the gas above the solution,  $c$  is the concentration of the solute and  $K_H$  is a constant with the dimensions of pressure divided by concentration [26]. The constant, known as the Henry's law constant, depends on the solute, the solvent and the temperature.

In particular, the "concentration" of the solute in solution may also be expressed as a mole fraction or as a molality [26].

So, for this study the Henry's Law Constant is as below:

$$K_H = p / x_{CO_2(\text{absorb})}$$

$$p = X_i P_T$$

Where

$K_H$  is the Henry's Law Constant

$p$  is the partial pressure

$x_{CO_2(\text{absorb})}$  is the mole fraction of  $CO_2$  gas in ionic liquid

$X_i$  is the mole fraction of  $CO_2$  in the gas mixture

## CHAPTER 4

### RESULTS AND DISCUSSION

#### 4.1 EXPERIMENTAL SETUP LEAKAGE TEST

Based on the results obtained (refer appendix 3), it shown the pressure is dropped within 5-8 hours. This indicated that there is a leakage occurred. Therefore, the test is run again but the pressure is introduced only from  $V_a$  to  $V_b$  to figure out the leakage along this point.

Based on the results obtained for the second run, it shown the pressure reading is constant for 7.15 hours. This indicated there is no leakage along this line. Therefore, the test is preceded to the next line between  $V_b$  to  $V_c$ .

In the third run the results of the pressure drop after more than 5 hours period of time. This indicated that there is leakage occurred along this line. After further investigation, few possibilities have been indentified as follow:

- a) Leakage between pressure cell and it's cover
- b) Leakage between the nut at pressure cell and the tubing to  $V_b$
- c) Leakage between  $V_b$  and the tubing

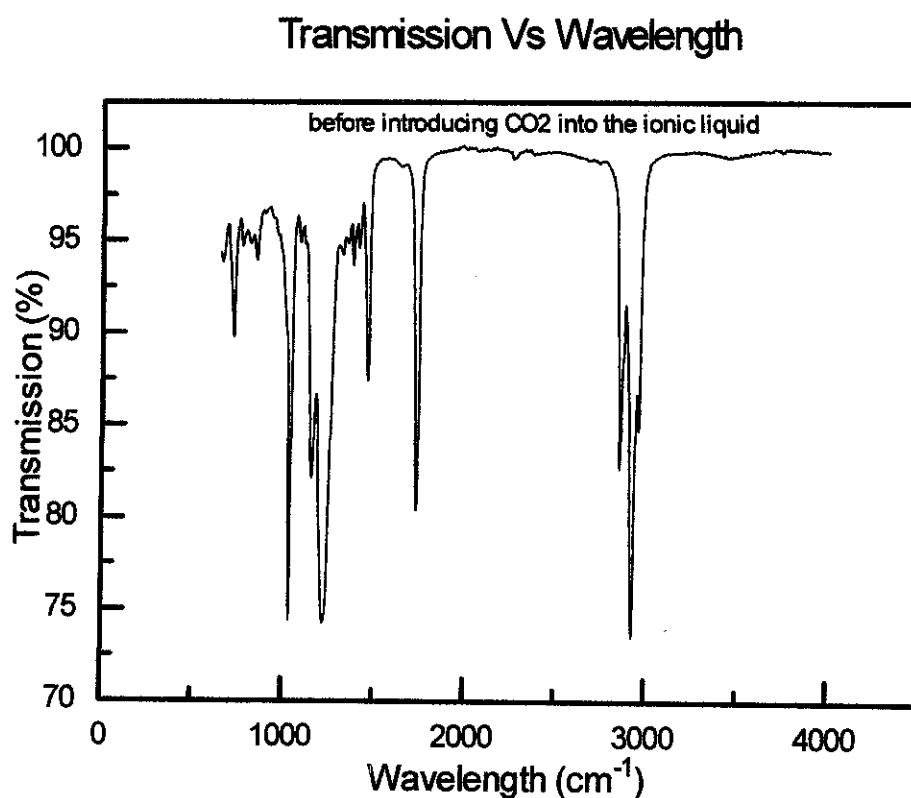
Actions have been taken to eliminate all the possibilities by putting thicker o-ring and hardly tighten all the connection.

The pressure still drop after the action taken. Therefore, again all the connection is tighten harder to make sure there is no leakage at all. The snoop also has been used to pre – check the leakage at every connection.

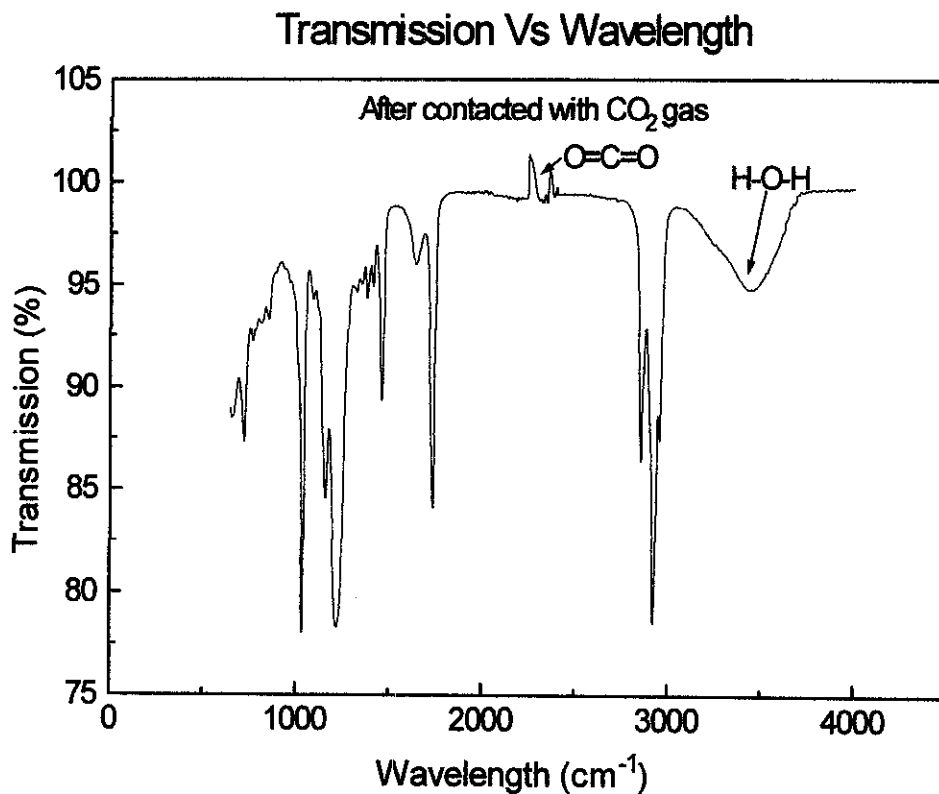
After that results showed the pressures are constant for 24 hours. So, this proved that there is no leakage from  $V_b$  to  $V_c$ . Therefore based on all tests that have been run, it is proved that the experimental setup is completely free from any leakage. This setup is ready to be used.

## 4.2 SPECTROSCOPY TEST

Based on the spectroscopy test result in figure 4.1 and 4.2, it shown the different trend for ionic liquid contacted with and without CO<sub>2</sub>. There are H-O-H and O=C=O bonds exists. Therefore, there degradation of the ionic structure occurred. Thus conclude that there is chemical absorption occurred between CO<sub>2</sub> and ionic liquid.



**Figure 4.1: Spectroscopy for Ionic Liquid without CO<sub>2</sub>**



**Figure 4.2: Spectroscopy for Ionic Liquid contacted with CO<sub>2</sub>**

### 4.3 VOLUME 1, V<sub>1</sub> DETERMINATION

#### 4.3.1 Initial Volume by Manual Calculation

$$V_{\text{initial}} = V_{\text{tube}} + V_{\text{vessel}}$$

$$V_{\text{tube}} = \pi r^2 h$$

$$= \pi \left( 0. \frac{635}{2} \right) 2 \times 32 \text{ cm}$$

$$= 10.1341 \text{ cm}^3$$

$$V_{\text{initial}} = V_{\text{tube}} + V_{\text{vessel}}$$

$$= 10.1341 \text{ cm}^3 + 75 \text{ cm}^3$$

$$= \underline{\underline{85.1341 \text{ cm}^3}}$$

### 4.3.2 Volume 1 by PV relationship

#### 4.2.1.1 First Trial

$$P_{\text{initial}} = 250 \text{ psi}$$

$$P_1 = 200 \text{ psi}$$

$$V_{\text{initial}} = 85.1341 \text{ cm}^3$$

$$P_{\text{initial}} V_{\text{initial}} = P_1 V_1$$

$$V_{\text{initial}} = P_{\text{initial}} V_{\text{initial}} / (P_1)$$

$$V_1 = (250)(85.1341) / (200)$$

$$V_1 = \underline{\underline{106.4176 \text{ cm}^3}}$$

#### 4.3.1.2 Second Trial

$$P_{\text{initial}} = 200 \text{ psi}$$

$$P_1 = 160 \text{ psi}$$

$$V_{\text{initial}} = 85.1341 \text{ cm}^3$$

$$P_{\text{initial}} V_{\text{initial}} = P_1 V_1$$

$$V_1 = P_{\text{initial}} V_{\text{initial}} / (P_1)$$

$$V_1 = (200)(85.1341) / (160)$$

$$V_1 = \underline{\underline{106.4176 \text{ cm}^3}}$$

#### 4.3.1.3 Third Trial

$$P_{\text{initial}} = 150 \text{ psi}$$

$$P_1 = 120 \text{ psi}$$

$$V_{\text{initial}} = 85.1341 \text{ cm}^3$$

$$P_{\text{initial}} V_{\text{initial}} = P_2 V_2$$

$$V_1 = P_{\text{initial}} V_{\text{initial}} / (P_2)$$

$$V_1 = (150)(85.1341) / (120)$$

$$V_1 = \underline{\underline{106.4176 \text{ cm}^3}}$$

### 4.3.2 Volume 1 by Manual Calculation

$$V_1 = V_{\text{tube}} + V_{\text{pressure cell}} + V_{\text{initial}} - V_{\text{stirrer}}$$

$$V_{\text{tube}} = \pi r^2 h$$

$$= \pi \left(0. \frac{635}{2}\right) 2 \times 36 \text{ cm}$$

$$= 10.7675 \text{ cm}^3$$

$$V_1 = V_{\text{tube}} + V_{\text{pressure cell}} + V_{\text{initial}} - V_{\text{stirrer}}$$

$$= 10.7675 \text{ cm}^3 + 12.5664 \text{ cm}^3 + 85.1341 \text{ cm}^3 - 2 \text{ cm}^3$$

$$= \underline{\underline{106.4680 \text{ cm}^3}} \sim \underline{\underline{106.4176 \text{ cm}^3}}$$

### 4.3.3 Determination of initial volume, $V_{\text{initial}}$ (backward method)

#### 4.3.3.1 First Trial

$$P_{\text{initial}} = 250 \text{ psi}$$

$$V_{\text{initial}} = ?$$

$$P_1 = 200 \text{ psi}$$

$$V_1 = 106.4176 \text{ cm}^3$$

$$P_{\text{initial}} V_{\text{initial}} = P_1 V_1$$

$$V_{\text{initial}} = P_1 V_1 / P_{\text{initial}}$$

$$= (200)(106.4176 \text{ cm}^3) / (250)$$

$$= \underline{\underline{85.1341 \text{ cm}^3}}$$

#### 4.3.3.2 Second Trial

$$P_{\text{initial}} = 200 \text{ psi}$$

$$V_{\text{initial}} = ?$$

$$P_1 = 160 \text{ psi}$$

$$V_1 = 106.4176 \text{ cm}^3$$

$$P_{\text{initial}} V_{\text{initial}} = P_1 V_1$$

$$V_{\text{initial}} = P_1 V_1 / P_{\text{initial}}$$

$$= (160)(106.4176 \text{ cm}^3) / (200)$$

$$= \underline{\underline{85.1341 \text{ cm}^3}}$$

### **4.3.3.3 Third Trial**

$$P_{\text{initial}} = 150 \text{ psi}$$

$$V_{\text{initial}} = ?$$

$$P_1 = 120 \text{ psi}$$

$$V_1 = 106.4176 \text{ cm}^3$$

$$P_{\text{initial}} V_{\text{initial}} = P_1 V_1$$

$$V_{\text{initial}} = P_1 V_1 / P_{\text{initial}}$$

$$= (120)(106.4176 \text{ cm}^3) / (150)$$

$$= \underline{\underline{85.1341 \text{ cm}^3}}$$

Based on the PV relation, it is verified that the  $V_{\text{initial}}$  is  $85.1341 \text{ cm}^3$  and the  $V_1$  without ionic liquid is  $106.4176 \text{ cm}^3$ .

Therefore,  $V_1$  after  $[\text{P}_{888}\text{C}_{10}\text{P}_{888}]$  docusate is added into the pressure cell is calculated as below:

$$V_1 = 106.4176 \text{ cm}^3 - V_{\text{il}}$$

$$V_{\text{il}} = \frac{2.0 \text{ g}}{(0.9665 \text{ g / cm}^3)}$$

$$= 2.0693 \text{ cm}^3$$

$$V_1 = (106.4176 - 2.0693) \text{ cm}^3$$

$$V_1 = \underline{\underline{104.3483 \text{ cm}^3}}$$

Where

$V_{\text{il}}$  is the volume of the ionic liquid ( $\text{m}^3$ )



## 4.4 SOLUBILITY MEASUREMENT

### 4.4.1 CO<sub>2</sub> Gas Mol Fraction and Molality

The solubility of CO<sub>2</sub> in [P<sub>888</sub>C<sub>10</sub>P<sub>888</sub>] docusate is measured at temperatures of (298.15, 303.15 and 308.15) K and pressures ranging from (15 to 25) bar. The detailed calculations of solubility data are presented in (Appendix 3). The solubility behavior of CO<sub>2</sub> in [P<sub>888</sub>C<sub>10</sub>P<sub>888</sub>] docusate with pressure is shown in Figure 4.3 till 4.8. It can be found that the solubility in terms of mol fraction and molality of CO<sub>2</sub> in [P<sub>888</sub>C<sub>10</sub>P<sub>888</sub>] docusate ionic liquid is increased with increasing of the pressure.

Based on the graphs obtained, it shown that mol fraction and molality of CO<sub>2</sub> gas in the ionic liquid is higher at high pressure compared to low pressure. Therefore, this indicated that the solubility of CO<sub>2</sub> is increased with the pressure.

This is because as the pressure is increased, the gas molecules are "forced" into the solution since this will best relieved the pressure that has been applied. The number of gas molecules is decreased while the number of CO<sub>2</sub> gas molecules dissolved in solution is increased. Thus, the amount of mol of CO<sub>2</sub> is increased.

**Table 4.1: Solubility Data at Different Temperatures**

| 298.15 K |                             |                                      | 303.15 K |                             |                                      | 308.15 K |                             |                                      |
|----------|-----------------------------|--------------------------------------|----------|-----------------------------|--------------------------------------|----------|-----------------------------|--------------------------------------|
| P (Mpa)  | X <sub>CO<sub>2</sub></sub> | m <sub>CO<sub>2</sub></sub> (mol/kg) | P (Mpa)  | X <sub>CO<sub>2</sub></sub> | m <sub>CO<sub>2</sub></sub> (mol/kg) | P (Mpa)  | X <sub>CO<sub>2</sub></sub> | m <sub>CO<sub>2</sub></sub> (mol/kg) |
| 1.99     | 0.6293                      | 1.0452                               | 2.00     | 0.5714                      | 0.8210                               | 2.01     | 0.4952                      | 0.6040                               |
| 1.59     | 0.5879                      | 0.8783                               | 1.60     | 0.5161                      | 0.6568                               | 1.61     | 0.4181                      | 0.4425                               |
| 1.19     | 0.5360                      | 0.7113                               | 1.20     | 0.4444                      | 0.4926                               | 1.20     | 0.3133                      | 0.2810                               |

Pressure Vs CO<sub>2</sub> Gas Mol Fraction

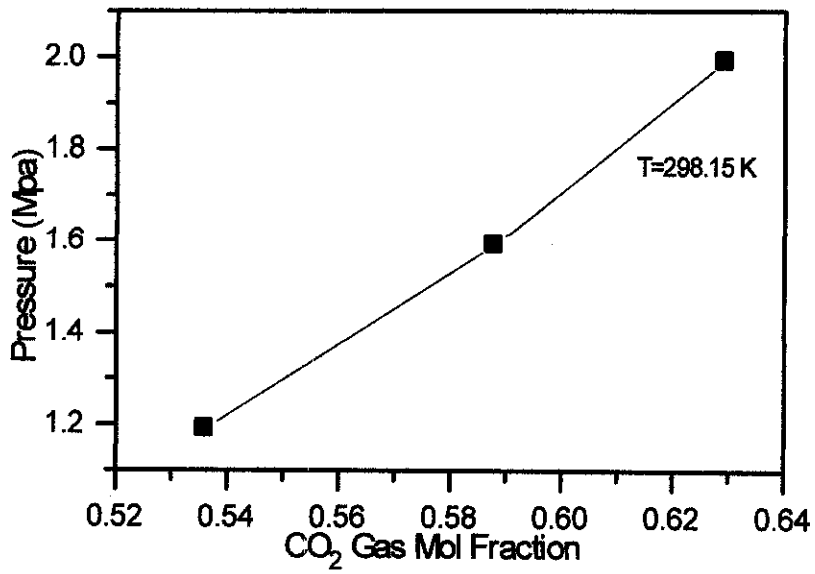


Figure 4.3: Graph Pressure vs CO<sub>2</sub> Mol Fraction at T=298.15 K

Pressure Vs CO<sub>2</sub> Gas Molality

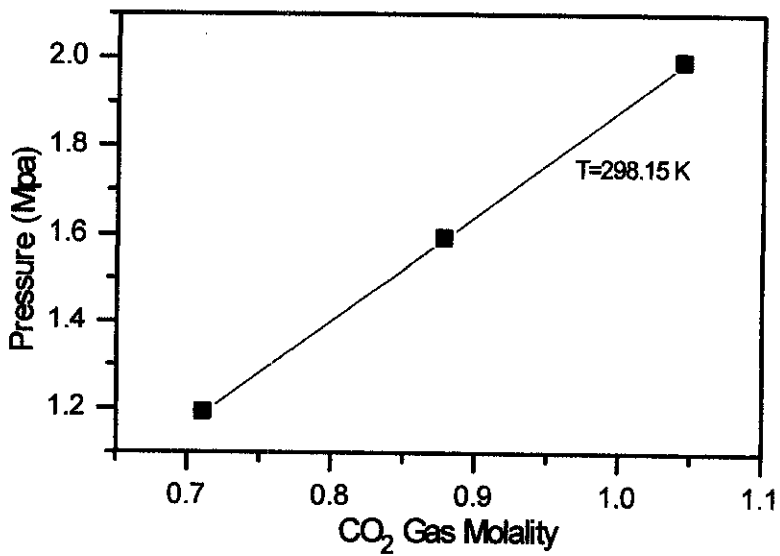


Figure 4.4: Graph Pressure vs CO<sub>2</sub> Gas Molality at T=298.15 K

Pressure Vs CO<sub>2</sub> Gas Mol Fraction

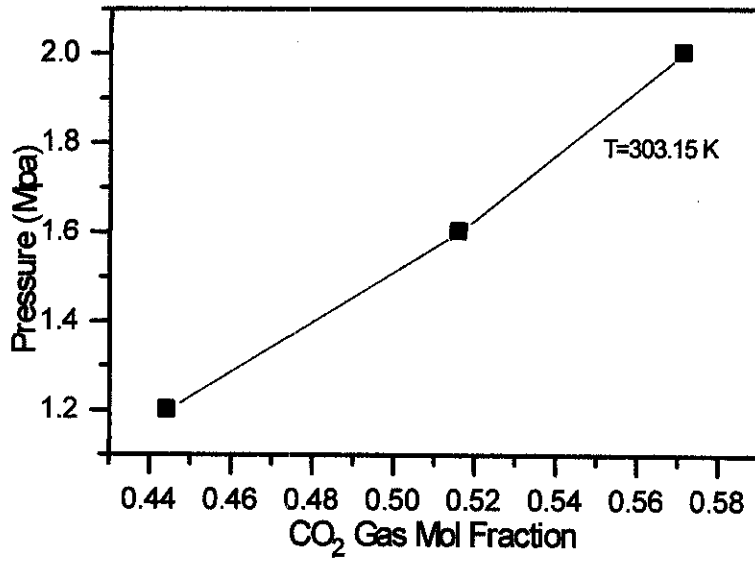


Figure 4.5: Graph Pressure vs CO<sub>2</sub> Mol Fraction at T=303.15 K

Pressure Vs CO<sub>2</sub> Gas Molality

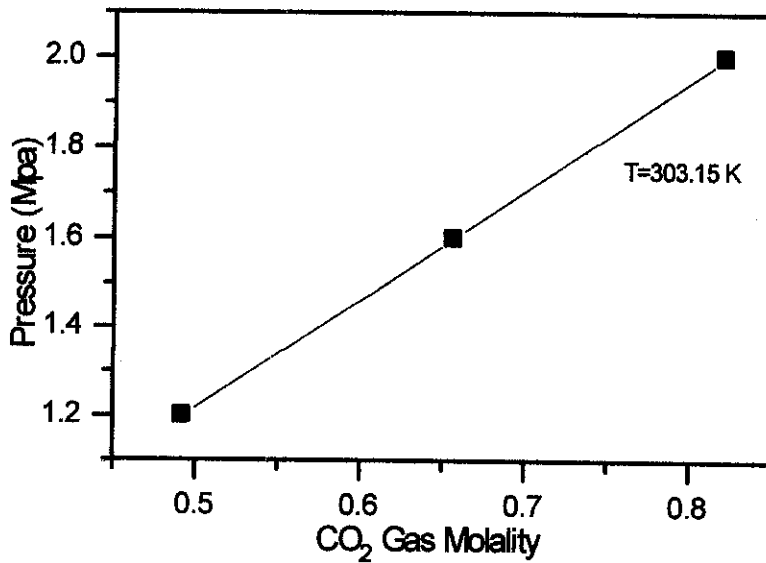
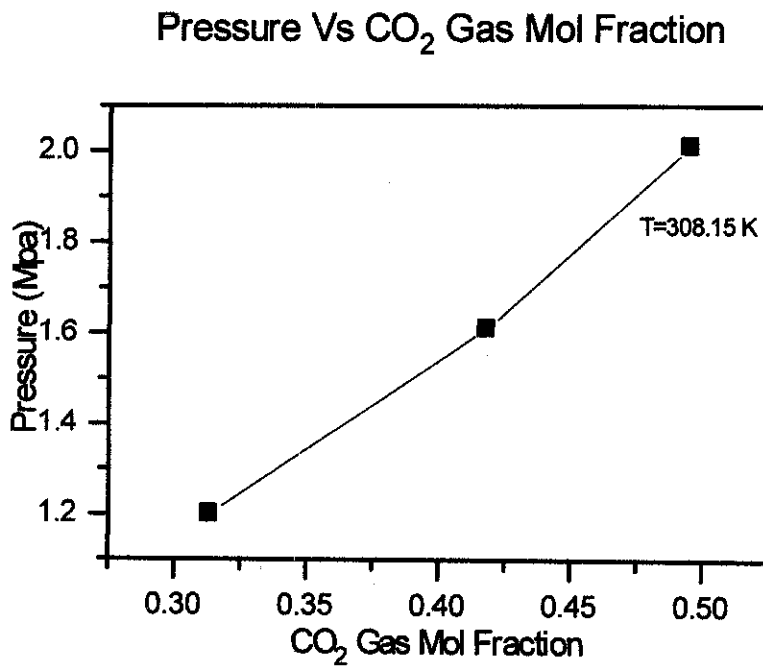
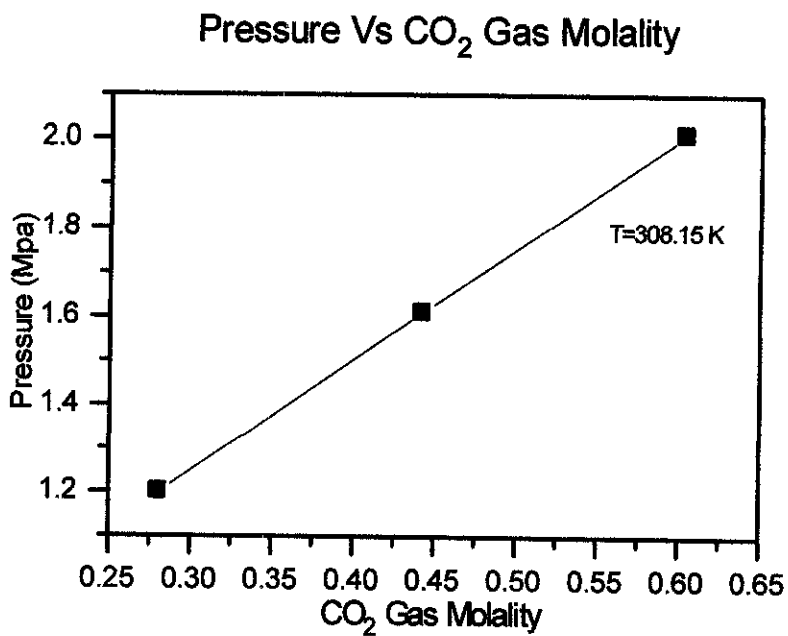


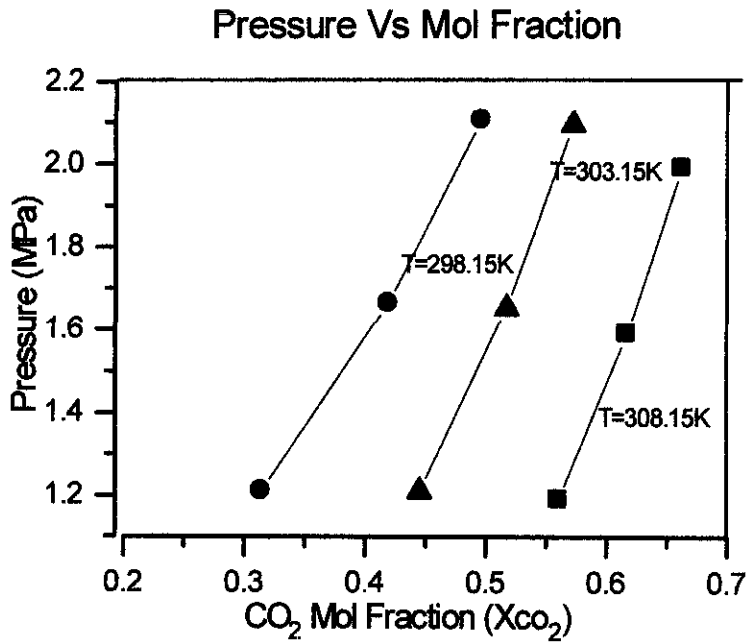
Figure 4.6: Graph Pressure vs CO<sub>2</sub> Gas Molality at T=303.15 K



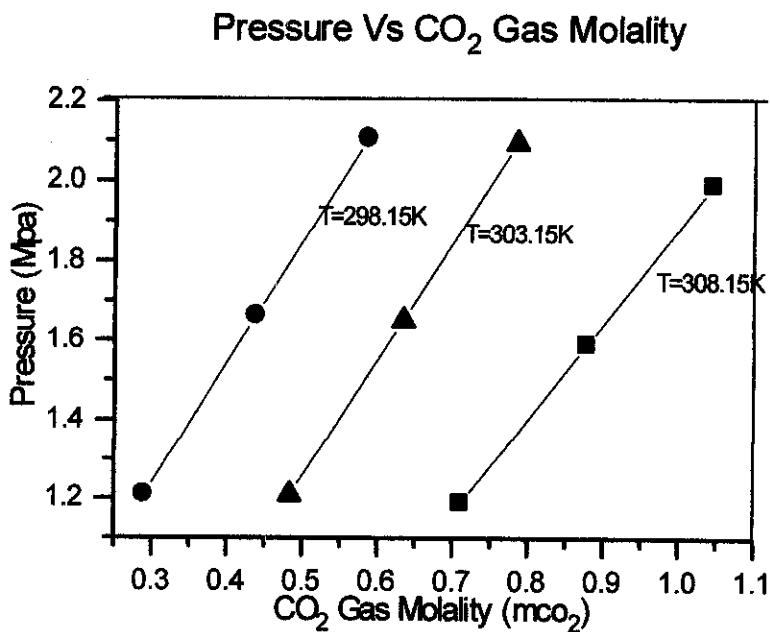
**Figure 4.7: Graph Pressure vs CO<sub>2</sub> Gas Mol Fraction at T=308.15 K**



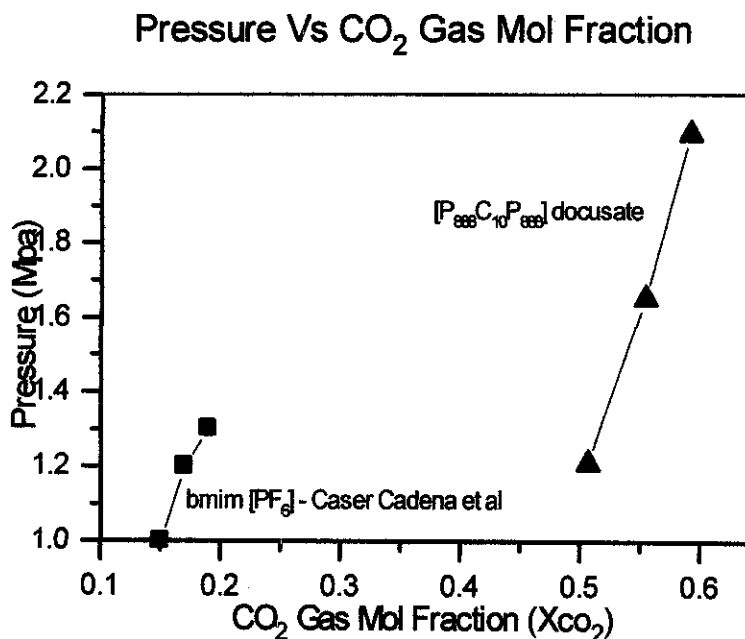
**Figure 4.8: Graph Pressure vs CO<sub>2</sub> Gas Molality at T=308.15 K**



**Figure 4.9: Pressure vs Mol Fraction at T= 298.15 K, T=303.15 K and T=308.15 K**



**Figure 4.10: Pressure vs CO<sub>2</sub> Gas Molality at T=298.15 K, T=303.15 K and T=308.15 K**



**Figure 4.11: Comparison with Literature Data for Pressure vs CO<sub>2</sub> Gas Mol Fraction at T=298.15 K**

Based on the comparison with the literature data of other ionic liquid, it shown that the mol graction for [bmim][PF<sub>6</sub>] is lesser than the mol fraction of this ionic liquid at temperature 298.15 K. This showed that this ionic can absorb more CO<sub>2</sub> compared to [bmim][PF<sub>6</sub>] which is more than 50% of CO<sub>2</sub> gas. This is due to the long alkyl chain structure of this ionic liquid it self. The CO<sub>2</sub> solubility increased with increasing chain length, and these results are consistent with those reported elsewhere [29]. It was thought that this may be due to entropic reasons, as the density of ionic liquids decreases with increasing alkyl chain length. Therefore, there may be more free volume within the longer chain ionic liquids.

#### 4.4.2 Henry's Law Constant at Different Temperature

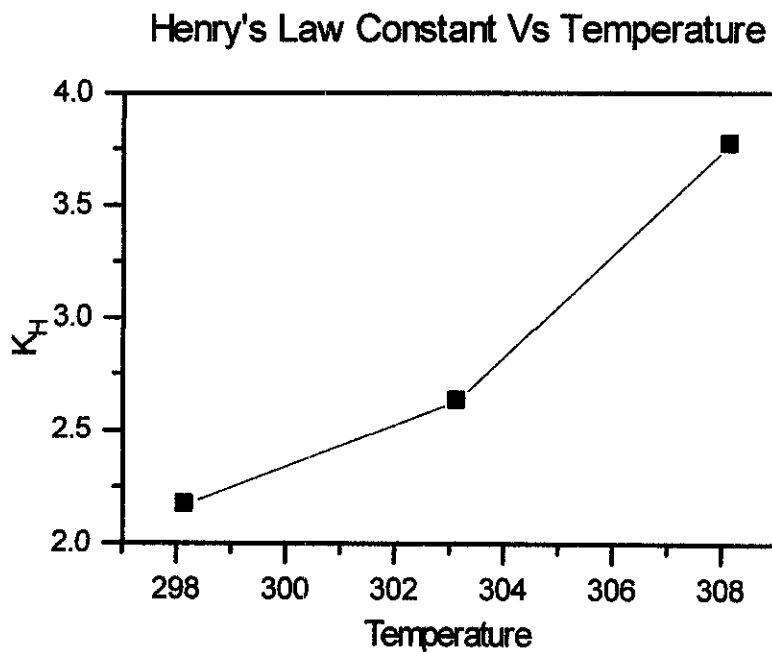
The Henry's law constants at different temperatures are shown in Table 4.2. From Table 4.2, it can be seen that the Henry's law constant of the studied systems increases with increasing temperature, which indicates the solubility of CO<sub>2</sub> decreases with increasing temperature.

As the temperature increases, the solubility of a CO<sub>2</sub> decreases. More CO<sub>2</sub> is present in a solution with a lower temperature compared to a solution with a higher temperature.

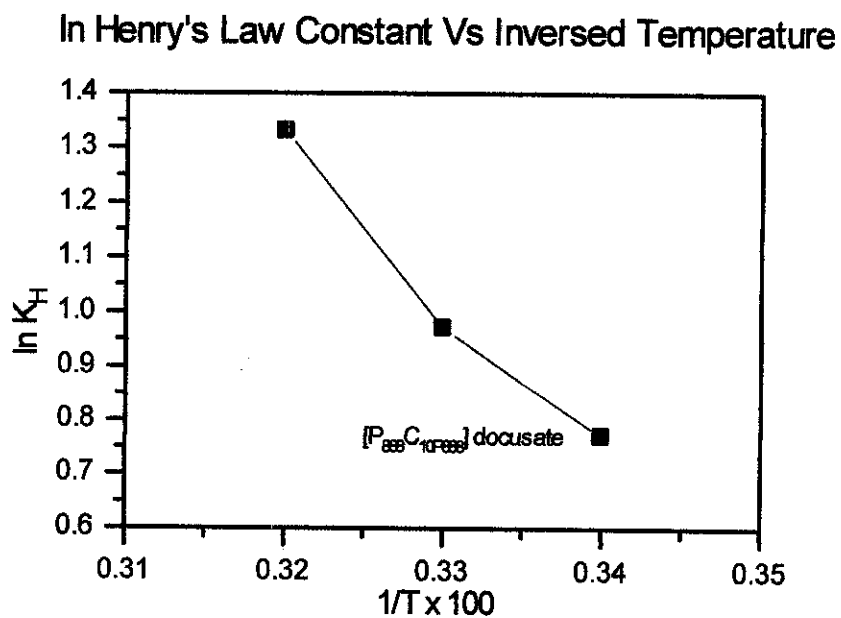
The reason for this CO<sub>2</sub> solubility relationship with temperature is very similar to the reason that vapor pressure increases with temperature. Increased temperature causes an increase in kinetic energy. The higher kinetic energy causes more motion in molecules which break intermolecular bonds and escape from solution.

**Table 4.2: Henry's Law Constant vs Temperature Data**

| T (K)  | K <sub>H</sub> (Mpa) | ln K <sub>H</sub> | 1/T (K <sup>-1</sup> ) x 100 |
|--------|----------------------|-------------------|------------------------------|
| 298.15 | 2.17                 | 0.77              | 0.34                         |
| 303.15 | 2.63                 | 0.97              | 0.33                         |
| 308.15 | 3.77                 | 1.33              | 0.32                         |



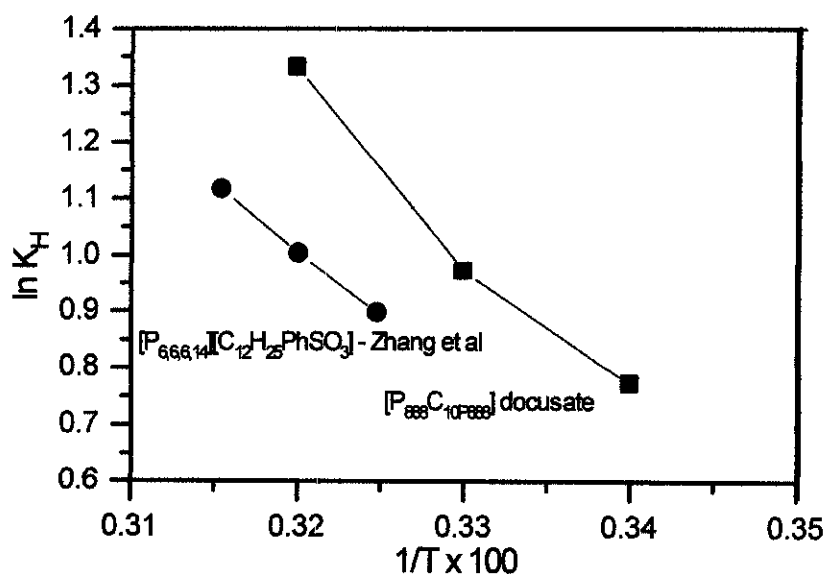
**Figure 4.12: Henry's Law Constant vs Temperature**



**Figure 4.13: The Logarithms of the Henry's Law Constant vs Inversed Temperature**



### In Henry's Law Constant Vs Inversed Temperature



**Figure 4.14: Comparison with Literature Data for Logarithms of the Henry's Law Constant vs Inverse Temperature**

Zhang et al shown that the Henry's law constant of  $[P_{6,6,6,14}][C_{12}H_{25}PhSO_3]$  is increases with increasing temperature, which indicates the solubility of  $CO_2$  decreases with increasing temperature. Based on the comparison above, it shown that the logarithms of Henry's Law Constant for  $[P_{888}C_{10}P_{888}]$  docusate is following the same trend as  $[P_{6,6,6,14}][C_{12}H_{25}PhSO_3]$ .

## **CHAPTER 5**

### **CONCLUSION AND RECOMMENDATIONS**

New experimental results for the solubility of CO<sub>2</sub> in the new synthesized ionic liquid [P<sub>888</sub>C<sub>10</sub>P<sub>888</sub>] docusate are presented for temperatures 298.15 K, 303.15 K, and 308.15 K and pressures ranging from 15 to 25 bars. Henry's law constants are determined from that solubility pressure data. The solubility pressures were correlated by means of extended Henry's law. The solubility results of new synthesized ionic liquid [P<sub>888</sub>C<sub>10</sub>P<sub>888</sub>] docusate are very important in many industrial applications.

Since most of the industrial processes operate at high pressure condition up to 100 bar (10 Mpa), the solubility measurement can be conducted at higher pressure up to 10 to 15 Mpa. Solubility measurement also can be conducted for nitrogen and methane gas because the solubility data is really important in the separation process of nitrogen and methane gas.

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**APPENDIX 1:**  
**PROJECT ACTIVITIES**

1. Research on related studies about CO<sub>2</sub> solubility in ionic liquids
2. Understanding the differences between difference types of ionic liquids
3. Understanding on ionic liquids properties and solubility of CO<sub>2</sub> in ionic liquids
4. Study on chemical properties of phosphonium-based ionic liquids
5. Understanding on how CO<sub>2</sub> solubility differs in phosphonium-based ionic liquids and imidazolium-based ionic liquid
6. Research and study on method of CO<sub>2</sub> solubility measurement
7. Study the factors that govern the solubility of CO<sub>2</sub> in ionic liquids
8. Decision on what will be focused in the project and method involved
9. Designing the equipment for solubility measurement
10. Consultation process about the equipment design with supervisor and fabricator
11. Confirmation of equipment with fabricator
12. Finalized all the equipments needed to set up the experiment
13. Set up the experimental apparatus for solubility measurement
14. Leakage test of the experimental setup
15. Determination of volume 1, V<sub>1</sub>
16. Solubility measurement of CO<sub>2</sub> in [P<sub>888</sub>C<sub>10</sub>P<sub>888</sub>] docusate

**APPENDIX 2: GANTT CHART AND KEY MILESTONE**

| No. | Detail/ Week                             | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |  |
|-----|--|---|---|---|---|---|---|---|---|---|----|----|----|----|----|--|
| 1   | Project Work Continue                    | ■ |   |   |   |   |   |   |   |   |    |    |    |    |    |  |
| 2   | Submission of Progress Report 1          |   |   |   | ● |   |   |   |   |   |    |    |    |    |    |  |
| 3   | Project Work Continue                    |   |   | ■ |   |   |   |   |   |   |    |    |    |    |    |  |
| 4   | Submission of Progress Report 2          |   |   |   |   |   |   |   |   |   |    |    |    |    |    |  |
| 5   | Seminar (compulsory)                     |   |   |   |   |   |   |   |   | ■ |    |    |    |    |    |  |
| 5   | Project work continue                    |   |   |   |   |   |   |   |   | ■ |    |    |    |    |    |  |
| 6   | Poster Exhibition                        |   |   |   |   |   |   |   |   |   |    |    |    |    |    |  |
| 7   | Submission of Dissertation (soft bound)  |   |   |   |   |   |   |   |   |   |    |    |    |    |    |  |
| 8   | Oral Presentation                        |   |   |   |   |   |   |   |   |   |    |    |    |    |    |  |
| 9   | Submission of Project Dissertation (Hard |   |   |   |   |   |   |   |   |   |    |    |    |    |    |  |

Mid-Semester Break

● Suggested milestone

■ Process

**APPENDIX 3:**  
**SOLUBILITY MEASUREMENT RESULTS AND CALCULATIONS**



### 3.1 Experimental Setup Leakage Test

#### 3.1.1 First Run

**Table 3.1: First Run of Leakage Test Results**

| <b>Date</b>   | <b>Time</b> | <b>Pressure Reading</b> |
|---------------|-------------|-------------------------|
| 23 March 2010 | 11.45 am    | 250 psi                 |
|               | 05.30 pm    | 220 psi                 |
| 24 March 2010 | 09.00 am    | 170 psi                 |

#### 3.1.2 Second Run

**Table 3.2: Second Run of Leakage Test Results**

| <b>Date</b>   | <b>Time</b> | <b>Pressure Reading</b> |
|---------------|-------------|-------------------------|
| 24 March 2010 | 10.15 am    | 255 psi                 |
|               | 05.30 pm    | 225 psi                 |

#### 3.1.3 Third Run

**Table 3.3: Third Run of Leakage Test Results**

| <b>Date</b>   | <b>Time</b> | <b>Pressure Reading</b> |
|---------------|-------------|-------------------------|
| 24 March 2010 | 05.40 pm    | 255 psi                 |
|               | 10.45 am    | 190 psi                 |

### 3.1.4 Fourth Run

**Table 3.4: Fourth Run of Leakage Test Results**

| <b>Date</b>   | <b>Time</b> | <b>Pressure Reading</b> |
|---------------|-------------|-------------------------|
| 26 March 2010 | 06.15 pm    | 255 psi                 |
| 29 March 2010 | 09.30 am    | 100 psi                 |
| 29 March 2010 | 09.35 am    | 250 psi                 |
|               | 03.10 pm    | 230 psi                 |
|               | 03.24 pm    | 255 psi                 |
| 30 March 2010 | 9.00 am     | 190 psi                 |

### 3.1.5 Fifth Run

**Table 3.5: Fourth Run of Leakage Test Results**

| <b>Date</b>   | <b>Time</b> | <b>Pressure Reading</b> |
|---------------|-------------|-------------------------|
| 30 March 2010 | 09.15 am    | 255 psi                 |
|               | 4.20 pm     | 255 psi                 |

### 3.2 Solubility Measurement at Stirring Speed (S) = 300 rpm and Temperature (T) = 298.15 K

#### 3.2.1 First Run

**Table 3.6: Pressure vs Time Data at Initial Pressure of 2 bar**

| <b>S= 300 rpm</b> |                 |
|-------------------|-----------------|
| <b>T=298.15K</b>  |                 |
| <b>Pi = 2 bar</b> |                 |
| <b>t (hours)</b>  | <b>Pf (bar)</b> |
| 0                 | 1.6             |
| 2                 | 1.6             |
| 4                 | 1.6             |
| 6                 | 1.6             |
| 8                 | 1.6             |
| 10                | 1.6             |
| 12                | 1.6             |
| 14                | 1.6             |
| 16                | 1.6             |
| 18                | 1.6             |
| 20                | 1.6             |
| 22                | 1.6             |
| 24                | 1.6             |

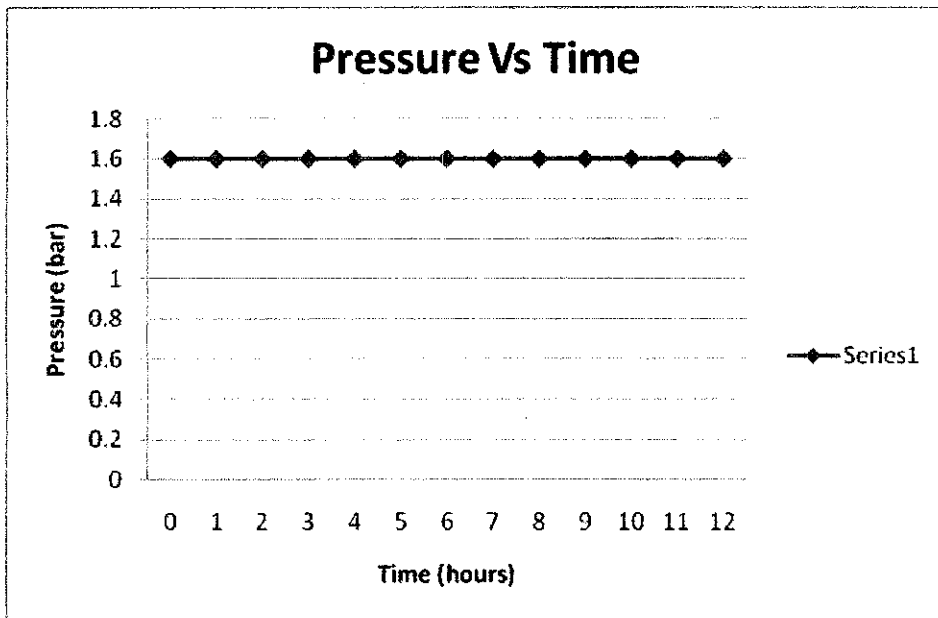
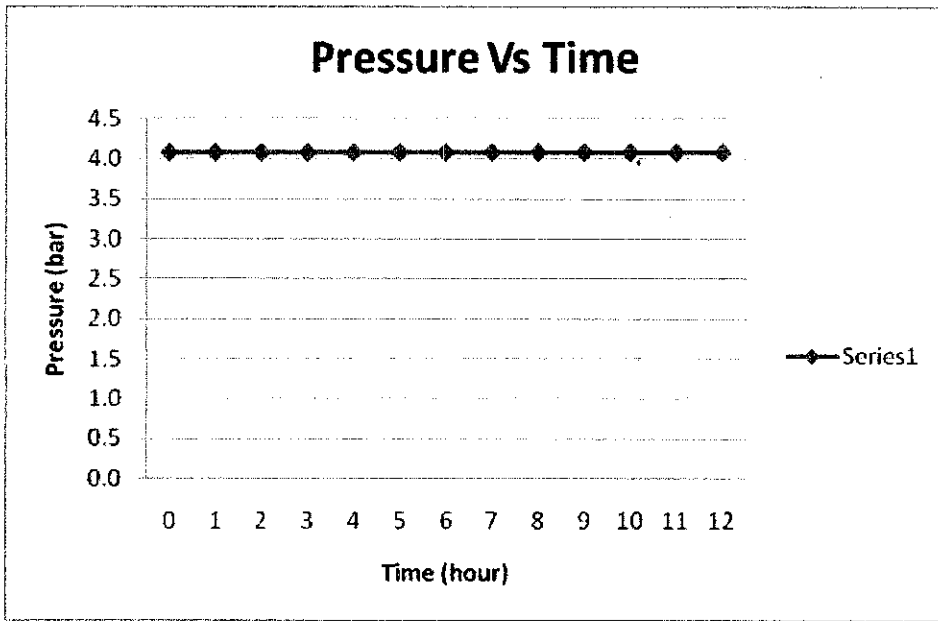


Figure 3.1: Graph Pressure vs Time at Initial Pressure of 2 bar

### 3.2.2 Second Run

Table 3.7: Pressure vs Time Data at Initial Pressure of 5 bar

| S=300 rpm  |          |
|------------|----------|
| T=298.15K  |          |
| Pi = 5 bar |          |
| t (hours)  | Pf (bar) |
| 0          | 4.1      |
| 2          | 4.1      |
| 4          | 4.1      |
| 6          | 4.1      |
| 8          | 4.1      |
| 10         | 4.1      |
| 12         | 4.1      |
| 14         | 4.1      |
| 16         | 4.1      |
| 18         | 4.1      |
| 20         | 4.1      |
| 22         | 4.1      |
| 24         | 4.1      |

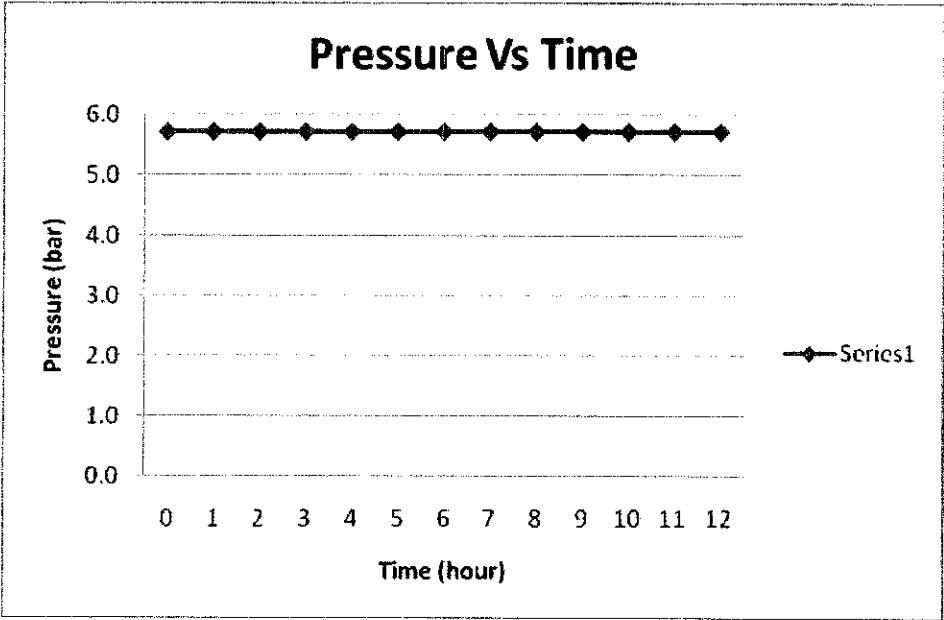


**Figure 3.2: Graph Pressure vs Time at Initial Pressure of 5 bar**

**3.2.3 Third Run**

**Table 3.8: Pressure vs Time Data at Initial Pressure of 7 bar**

| <b>S=300 rpm</b>  |                 |
|-------------------|-----------------|
| <b>T=298.15K</b>  |                 |
| <b>Pi = 7 bar</b> |                 |
| <b>t (hours)</b>  | <b>Pf (bar)</b> |
| 0                 | 5.7             |
| 2                 | 5.7             |
| 4                 | 5.7             |
| 6                 | 5.7             |
| 8                 | 5.7             |
| 10                | 5.7             |
| 12                | 5.7             |
| 14                | 5.7             |
| 16                | 5.7             |
| 18                | 5.7             |
| 20                | 5.7             |
| 22                | 5.7             |
| 24                | 5.7             |



**Figure 3.3: Graph Pressure vs Time at Initial Pressure of 7 bar**

### 3.3 Solubility Measurement at Different Stirring Speed (S), Initial Pressure (P<sub>i</sub>) and Temperature (T) = 298.15 K

#### 3.3.1 First Run P<sub>i</sub> = 15 bar

**Table 3.9: Solubility of CO<sub>2</sub> in Ionic Liquid at T=298.15 K and P<sub>i</sub>=15 bar**

| S=300 rpm               |          |                     |                |                |                           |  |                                      |
|-------------------------|----------|---------------------|----------------|----------------|---------------------------|--|--------------------------------------|
| T= 298.15 K             |          |                     |                |                |                           |  |                                      |
| P <sub>i</sub> = 15 bar |          |                     |                |                |                           |  |                                      |
| hours)                  | Pf (bar) | P <sub>needed</sub> | n <sub>1</sub> | n <sub>2</sub> | n <sub>absorb</sub> (mol) | X <sub>CO<sub>2</sub></sub> (fraction) | m <sub>CO<sub>2</sub></sub> (mol/kg) |
| 0                       | 12.2     | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 2                       | 12.2     | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 4                       | 12.2     | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 6                       | 12.2     | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 8                       | 12.2     | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 10                      | 12.2     | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 12                      | 12.2     | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 14                      | 12.2     | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 16                      | 12.2     | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 18                      | 12.2     | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 20                      | 12.2     | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 22                      | 12.1     | 0.1                 | 0.05151        | 0.05093        | 0.00058                   | 0.32046                                | 0.29039                              |
| 24                      | 11.9     | 0.3                 | 0.05151        | 0.05009        | 0.00142                   | 0.53600                                | 0.71132                              |

$$P_{\text{needed}} = 12.2 \text{ bar} - 11.9 \text{ bar}$$

$$P_{\text{needed}} = 0.3 \text{ bar}$$

$$n_1 = \frac{(12.2 \text{ bar} \times 100000 \text{ pa / bar}) \times (104.3483 \text{ cm}^3 \times 0.000001 \text{ m}^3 / \text{cm}^3)}{(298.15\text{K}) (8.314472 \text{ J / K.mol})}$$

$$n_1 = 0.05151 \text{ mol CO}_2$$

$$n_2 = \frac{(11.9 \text{ bar} \times 100000 \text{ pa / bar}) \times (104.3483 \text{ cm}^3 \times 0.000001 \text{ m}^3 / \text{cm}^3)}{(298.15\text{K}) (8.314472 \text{ J / K.mol})}$$

$$n_2 = 0.05009 \text{ mol CO}_2$$

$$n_{\text{absorb}} = n_1 - n_2$$

$$= (0.05151 - 0.05009) \text{ mol CO}_2$$

$$= 0.00142 \text{ mol CO}_2$$

$$X_{\text{CO}_2} = (0.00142 \text{ mol CO}_2) / (0.00142 \text{ mol CO}_2 + 0.001231527 \text{ mol ionic liquid})$$

$$X_{\text{CO}_2} = 0.53600 \text{ mol CO}_2$$

$$m_{\text{CO}_2} = 0.00142 \text{ mol CO}_2 / 0.002 \text{ kg of ionic liquid}$$

$$m_{\text{CO}_2} = 0.71132 \text{ mol CO}_2 / \text{kg ionic liquid}$$

### 3.3.2 Second Run $P_1 = 20$ bar

Table 3.10: Solubility of CO<sub>2</sub> in Ionic Liquid at T=298.15 K and P<sub>f</sub>=20 bar

| S=500 rpm   |          |         |         |         |               |                             |                           |
|-------------|----------|---------|---------|---------|---------------|-----------------------------|---------------------------|
| T= 298.15 K |          |         |         |         |               |                             |                           |
| Pi = 20 bar |          |         |         |         |               |                             |                           |
| hours       | Pf (bar) | Pneeded | n1      | n2      | nabsorb (mol) | Xco <sub>2</sub> (fraction) | mco <sub>2</sub> (mol/kg) |
| 0           | 16.3     | 0       | 0       | 0       | 0             | 0                           | 0                         |
| 2           | 16.3     | 0       | 0       | 0       | 0             | 0                           | 0                         |
| 4           | 16.3     | 0       | 0       | 0       | 0             | 0                           | 0                         |
| 6           | 16.3     | 0       | 0       | 0       | 0             | 0                           | 0                         |
| 8           | 16.3     | 0       | 0       | 0       | 0             | 0                           | 0                         |
| 10          | 16.3     | 0       | 0       | 0       | 0             | 0                           | 0                         |
| 12          | 16.3     | 0       | 0       | 0       | 0             | 0                           | 0                         |
| 14          | 16.3     | 0       | 0       | 0       | 0             | 0                           | 0                         |
| 16          | 16.3     | 0       | 0       | 0       | 0             | 0                           | 0                         |
| 18          | 16.3     | 0       | 0       | 0       | 0             | 0                           | 0                         |
| 20          | 16.2     | 0.1     | 0.06869 | 0.06819 | 0.00049       | 0.28618                     | 0.24687                   |
| 22          | 16.1     | 0.2     | 0.06869 | 0.06777 | 0.00091       | 0.42618                     | 0.45734                   |
| 24          | 15.9     | 0.4     | 0.06869 | 0.06693 | 0.00176       | 0.58785                     | 0.87827                   |

$$P_{\text{needed}} = 16.3 \text{ bar} - 15.9 \text{ bar}$$



$$P_{\text{needed}} = 0.4 \text{ bar}$$

$$n_1 = \frac{(16.3 \text{ bar} \times 100000 \text{ pa} / \text{bar}) \times (104.3483 \text{ cm}^3 \times 0.000001 \text{ m}^3 / \text{cm}^3)}{(303.15\text{K}) (8.314472 \text{ J} / \text{K.mol})}$$

$$n_1 = 0.06869 \text{ mol CO}_2$$

$$n_2 = \frac{(15.9 \text{ bar} \times 100000 \text{ pa} / \text{bar}) \times (104.3483 \text{ cm}^3 \times 0.000001 \text{ m}^3 / \text{cm}^3)}{(303.15\text{K}) (8.314472 \text{ J} / \text{K.mol})}$$

$$n_2 = 0.06693 \text{ mol CO}_2$$

$$n_{\text{absorb}} = n_1 - n_2$$

$$= (0.06869 - 0.06693) \text{ mol CO}_2$$

$$= 0.00176 \text{ mol CO}_2$$

$$X_{\text{CO}_2} = (0.00176 \text{ mol CO}_2) / (0.00176 \text{ mol CO}_2 + 0.001231527 \text{ mol ionic liquid})$$

$$X_{\text{CO}_2} = \mathbf{0.58785 \text{ mol CO}_2}$$

$$m_{\text{CO}_2} = 0.00176 \text{ mol CO}_2 / 0.002 \text{ kg of ionic liquid}$$

$$m_{\text{CO}_2} = \mathbf{0.87827 \text{ mol CO}_2 / \text{kg ionic liquid}}$$

### 3.3.3 Third Run $P_i = 25$ bar

**Table 3.11: Solubility of CO<sub>2</sub> in Ionic Liquid at  $P_i=25$  bar**

| S=700 rpm               |                      |                     |                |                |                           |  |                                      |
|-------------------------|----------------------|---------------------|----------------|----------------|---------------------------|--|--------------------------------------|
| T= 298.15 K             |                      |                     |                |                |                           |  |                                      |
| P <sub>i</sub> = 25 bar |                      |                     |                |                |                           |  |                                      |
| hours)                  | P <sub>f</sub> (bar) | P <sub>needed</sub> | n <sub>1</sub> | n <sub>2</sub> | n <sub>absorb</sub> (mol) | X <sub>co<sub>2</sub></sub> (fraction) | m <sub>co<sub>2</sub></sub> (mol/kg) |
| 0                       | 20.4                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 2                       | 20.4                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 4                       | 20.4                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 6                       | 20.4                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 8                       | 20.4                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 10                      | 20.4                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 12                      | 20.4                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 14                      | 20.4                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 16                      | 20.4                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 18                      | 20.4                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 24                      | 20.3                 | 0.1                 | 0.08586        | 0.08545        | 0.00041                   | 0.24826                                | 0.20335                              |
| 24                      | 20.1                 | 0.3                 | 0.08586        | 0.08461        | 0.00125                   | 0.50344                                | 0.62429                              |
| <b>24</b>               | <b>19.9</b>          | <b>0.5</b>          | <b>0.08586</b> | <b>0.08377</b> | <b>0.00209</b>            | <b>0.62928</b>                         | <b>1.04522</b>                       |

$$P_{needed} = 20.4 \text{ bar} - 19.9 \text{ bar}$$

$$P_{needed} = 0.5 \text{ bar}$$

$$n_1 = \frac{(20.4 \text{ bar} \times 100000 \text{ pa / bar}) \times (104.3483 \text{ cm}^3 \times 0.000001 \text{ m}^3 / \text{cm}^3)}{(298.15\text{K}) (8.314472 \text{ J / K.mol})}$$

$$n_1 = 0.08586 \text{ mol CO}_2$$

$$n_2 = \frac{(19.9 \text{ bar} \times 100000 \text{ pa / bar}) \times (104.3483 \text{ cm}^3 \times 0.000001 \text{ m}^3 / \text{cm}^3)}{(298.15\text{K}) (8.314472 \text{ J / K.mol})}$$

$$n_2 = 0.08377 \text{ mol CO}_2$$

$$n_{absorb} = n_1 - n_2$$

$$= (0.08586 - 0.08377) \text{ mol CO}_2$$

$$= 0.00209 \text{ mol CO}_2$$

$$X_{\text{CO}_2} = (0.00209 \text{ mol CO}_2) / (0.00209 \text{ mol CO}_2 + 0.001231527 \text{ mol ionic liquid})$$

$$X_{\text{CO}_2} = \mathbf{0.62928 \text{ mol CO}_2}$$

$$m_{\text{CO}_2} = 0.62928 \text{ mol CO}_2 / 0.002 \text{ kg of ionic liquid}$$

$$m_{\text{CO}_2} = \mathbf{1.0452 \text{ mol CO}_2 / \text{kg ionic liquid}}$$

**3.4 Solubility Measurement at Different Stirring Speed (S), Initial Pressure (P<sub>i</sub>) and Temperature (T) = 303.15 K**

**3.4.1 First Run P<sub>i</sub> = 15 bar**

**Table 3.12: Solubility of CO<sub>2</sub> in Ionic Liquid at T = 303.15 K and P<sub>i</sub>=15 bar**

| <b>S=300 rpm</b>              |                                |                           |                      |                      |                                 |  |  |
|-------------------------------|--------------------------------|---------------------------|----------------------|----------------------|---------------------------------|--|--|
| <b>T= 303.15 K</b>            |                                |                           |                      |                      |                                 |  |  |
| <b>P<sub>i</sub> = 15 bar</b> |                                |                           |                      |                      |                                 |  |  |
| <b>(hours)</b>                | <b>P<sub>f</sub><br/>(bar)</b> | <b>P<sub>needed</sub></b> | <b>n<sub>1</sub></b> | <b>n<sub>2</sub></b> | <b>n<sub>absorb</sub> (mol)</b> | <b>X<sub>CO<sub>2</sub></sub> (fraction)</b> | <b>m<sub>CO<sub>2</sub></sub> (mol/kg)</b> |
| 0                             | 12.2                           | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 2                             | 12.2                           | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 4                             | 12.2                           | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 6                             | 12.2                           | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 8                             | 12.2                           | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 10                            | 12.2                           | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 12                            | 12.2                           | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 14                            | 12.2                           | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 16                            | 12.2                           | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 18                            | 12.2                           | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 20                            | 12.2                           | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 22                            | 12.2                           | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| <b>24</b>                     | <b>12.0</b>                    | <b>0.2</b>                | <b>0.05066</b>       | <b>0.04968</b>       | <b>0.00099</b>                  | <b>0.44444</b>                               | <b>0.49259</b>                             |

### 3.4.2 First Run $P_i = 20$ bar

Table 3.13: Solubility of  $\text{CO}_2$  in Ionic Liquid at  $T = 303.15$  K and  $P_i = 20$  bar

| S=500 rpm               |                      |                     |                |                |                           |  |                                      |
|-------------------------|----------------------|---------------------|----------------|----------------|---------------------------|--|--------------------------------------|
| T= 303.15 K             |                      |                     |                |                |                           |  |                                      |
| P <sub>i</sub> = 20 bar |                      |                     |                |                |                           |  |                                      |
| (hours)                 | P <sub>f</sub> (bar) | P <sub>needed</sub> | n <sub>1</sub> | n <sub>2</sub> | n <sub>absorb</sub> (mol) | X <sub>CO<sub>2</sub></sub> (fraction) | m <sub>CO<sub>2</sub></sub> (mol/kg) |
| 0                       | 16.3                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 2                       | 16.3                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 4                       | 16.3                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 6                       | 16.3                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 8                       | 16.3                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 10                      | 16.3                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 12                      | 16.3                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 14                      | 16.3                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 16                      | 16.3                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 18                      | 16.3                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 20                      | 16.3                 | 0                   | 0              | 0              | 0                         | 0                                      | 0                                    |
| 22                      | 16.2                 | 0.1                 | 0.06755        | 0.06707        | 0.00049                   | 0.28280                                | 0.24280                              |
| 24                      | 16.0                 | 0.3                 | 0.06755        | 0.06624        | 0.00131                   | 0.51612                                | 0.65679                              |

### 3.4.3 Third Run $P_i = 25$ bar

**Table 3.14: Solubility of CO<sub>2</sub> in Ionic Liquid at T = 303.15 K and  $P_i=25$  bar**

| <b>S=700 rpm</b>                 |                 |                |                |                |                                 |                                   |                                 |
|----------------------------------|-----------------|----------------|----------------|----------------|---------------------------------|-----------------------------------|---------------------------------|
| <b>T= 303.15 K</b>               |                 |                |                |                |                                 |                                   |                                 |
| <b><math>P_i = 25</math> bar</b> |                 |                |                |                |                                 |                                   |                                 |
| <b>(hours)</b>                   | <b>Pf (bar)</b> | <b>Pneeded</b> | <b>n1</b>      | <b>n2</b>      | <b>n<sub>absorb</sub> (mol)</b> | <b>X<sub>co2</sub> (fraction)</b> | <b>m<sub>co2</sub> (mol/kg)</b> |
| 0                                | 20.4            | 0              | 0              | 0              | 0                               | 0                                 | 0                               |
| 2                                | 20.4            | 0              | 0              | 0              | 0                               | 0                                 | 0                               |
| 4                                | 20.4            | 0              | 0              | 0              | 0                               | 0                                 | 0                               |
| 6                                | 20.4            | 0              | 0              | 0              | 0                               | 0                                 | 0                               |
| 8                                | 20.4            | 0              | 0              | 0              | 0                               | 0                                 | 0                               |
| 10                               | 20.4            | 0              | 0              | 0              | 0                               | 0                                 | 0                               |
| 12                               | 20.4            | 0              | 0              | 0              | 0                               | 0                                 | 0                               |
| 14                               | 20.4            | 0              | 0              | 0              | 0                               | 0                                 | 0                               |
| 16                               | 20.4            | 0              | 0              | 0              | 0                               | 0                                 | 0                               |
| 18                               | 20.4            | 0              | 0              | 0              | 0                               | 0                                 | 0                               |
| <b>20</b>                        | <b>20.3</b>     | <b>0.1</b>     | <b>0.08444</b> | <b>0.08404</b> | <b>0.00040</b>                  | <b>0.24517</b>                    | <b>0.20000</b>                  |
| <b>22</b>                        | <b>20.2</b>     | <b>0.2</b>     | <b>0.08444</b> | <b>0.08363</b> | <b>0.00081</b>                  | <b>0.39794</b>                    | <b>0.40699</b>                  |
| <b>24</b>                        | <b>20.0</b>     | <b>0.4</b>     | <b>0.08444</b> | <b>0.08280</b> | <b>0.00164</b>                  | <b>0.57142</b>                    | <b>0.82099</b>                  |

**3.5 Solubility Measurement at Different Stirring Speed (S), Initial Pressure (P<sub>i</sub>) and Temperature (T) = 308.15 K**

**3.5.1 First Run P<sub>i</sub> = 15 bar**

**Table 3.15: Solubility of CO<sub>2</sub> in Ionic Liquid at T = 308.15 K and P<sub>f</sub>=15 bar**

| <b>S=300 rpm</b>              |                            |                           |                      |                      |                                 |  |  |
|-------------------------------|----------------------------|---------------------------|----------------------|----------------------|---------------------------------|--|--|
| <b>T= 308.15 K</b>            |                            |                           |                      |                      |                                 |  |  |
| <b>P<sub>i</sub> = 15 bar</b> |                            |                           |                      |                      |                                 |  |  |
| <b>t (hours)</b>              | <b>P<sub>f</sub> (bar)</b> | <b>P<sub>needed</sub></b> | <b>n<sub>1</sub></b> | <b>n<sub>2</sub></b> | <b>n<sub>absorb</sub> (mol)</b> | <b>X<sub>co<sub>2</sub></sub> (fraction)</b> | <b>m<sub>co<sub>2</sub></sub> (mol/kg)</b> |
| 0                             | 12.2                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 2                             | 12.2                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 4                             | 12.2                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 6                             | 12.2                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 8                             | 12.2                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 10                            | 12.2                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 12                            | 12.2                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 14                            | 12.2                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 16                            | 12.2                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 18                            | 12.2                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 20                            | 12.2                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 22                            | 12.2                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| <b>24</b>                     | <b>12.1</b>                | <b>0.1</b>                | <b>0.04984</b>       | <b>0.04928</b>       | <b>0.00056</b>                  | <b>0.31332</b>                               | <b>0.28096</b>                             |

### 3.5.2 Second Run $P_i = 20$ bar

**Table 3.16: Solubility of CO<sub>2</sub> in Ionic Liquid at T = 308.15 K and  $P_f=20$  bar**

| <b>S=500 rpm</b>              |                            |                           |                      |                      |                                 |  |  |
|-------------------------------|----------------------------|---------------------------|----------------------|----------------------|---------------------------------|--|--|
| <b>T= 308.15 K</b>            |                            |                           |                      |                      |                                 |  |  |
| <b>P<sub>i</sub> = 20 bar</b> |                            |                           |                      |                      |                                 |  |  |
| <b>t (hours)</b>              | <b>P<sub>f</sub> (bar)</b> | <b>P<sub>needed</sub></b> | <b>n<sub>1</sub></b> | <b>n<sub>2</sub></b> | <b>n<sub>absorb</sub> (mol)</b> | <b>X<sub>co<sub>2</sub></sub> (fraction)</b> | <b>m<sub>co<sub>2</sub></sub> (mol/kg)</b> |
| 0                             | 16.3                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 2                             | 16.3                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 4                             | 16.3                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 6                             | 16.3                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 8                             | 16.3                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 10                            | 16.3                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 12                            | 16.3                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 14                            | 16.3                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 16                            | 16.3                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 18                            | 16.3                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| 20                            | 16.3                       | 0                         | 0                    | 0                    | 0                               | 0  | 0  |
| <b>22</b>                     | <b>16.2</b>                | <b>0.1</b>                | <b>0.06646</b>       | <b>0.06598</b>       | <b>0.00048</b>                  | <b>0.27949</b>                               | <b>0.23886</b>                             |
| <b>24</b>                     | <b>16.1</b>                | <b>0.2</b>                | <b>0.06646</b>       | <b>0.06557</b>       | <b>0.00088</b>                  | <b>0.41814</b>                               | <b>0.44250</b>                             |



### 3.5.3 Third Run $P_i = 25$ bar

**Table 3.17: Solubility of CO<sub>2</sub> in Ionic Liquid at T = 308.15 K and  $P_i=25$  bar**

| <b>S=700 rpm</b>   |                 |                |           |           |                                 |                                   |                                 |
|--------------------|-----------------|----------------|-----------|-----------|---------------------------------|-----------------------------------|---------------------------------|
| <b>T= 308.15 K</b> |                 |                |           |           |                                 |                                   |                                 |
| <b>Pi = 25 bar</b> |                 |                |           |           |                                 |                                   |                                 |
| <b>t (hours)</b>   | <b>Pf (bar)</b> | <b>Pneeded</b> | <b>n1</b> | <b>n2</b> | <b>n<sub>absorb</sub> (mol)</b> | <b>X<sub>co2</sub> (fraction)</b> | <b>m<sub>co2</sub> (mol/kg)</b> |
| 0                  | 20.4            | 0              | 0         | 0         | 0                               | 0                                 | 0                               |
| 2                  | 20.4            | 0              | 0         | 0         | 0                               | 0                                 | 0                               |
| 4                  | 20.4            | 0              | 0         | 0         | 0                               | 0                                 | 0                               |
| 6                  | 20.4            | 0              | 0         | 0         | 0                               | 0                                 | 0                               |
| 8                  | 20.4            | 0              | 0         | 0         | 0                               | 0                                 | 0                               |
| 10                 | 20.4            | 0              | 0         | 0         | 0                               | 0                                 | 0                               |
| 12                 | 20.4            | 0              | 0         | 0         | 0                               | 0                                 | 0                               |
| 14                 | 20.4            | 0              | 0         | 0         | 0                               | 0                                 | 0                               |
| 16                 | 20.4            | 0              | 0         | 0         | 0                               | 0                                 | 0                               |
| 18                 | 20.4            | 0              | 0         | 0         | 0                               | 0                                 | 0                               |
| 20                 | 20.3            | 0.1            | 0.08307   | 0.08268   | 0.00039                         | 0.24215                           | 0.19675                         |
| 22                 | 20.2            | 0.2            | 0.08307   | 0.08227   | 0.00080                         | 0.39403                           | 0.40039                         |
| 24                 | 20.1            | 0.3            | 0.08307   | 0.08186   | 0.00121                         | 0.49519                           | 0.60403                         |

## APPENDIX 4: HENRY'S LAW CONSTANTS

**Table 4.1: Henry's Law Constant at 298.15 K**

| S=300 rpm<br>T= 298.15 K<br>Pi = 15 bar |         |                |         |          |         |             |
|---|---------|----------------|---------|----------|---------|-------------|
| Ptotal (Mpa)                            | Xi      | Ppartial (Mpa) | Xco2    | KH (Mpa) | ln KH   | 100/T (k-1) |
| 1.19000                                 | 0.97600 | 1.16145        | 0.53600 | 2.16686  | 0.77328 | 0.33540     |

**Table 4.2: Henry's Law Constant at 303.15 K**

| S=300 rpm<br>T= 303.15 K<br>Pi = 15 bar |         |                |         |          |         |             |
|---|---------|----------------|---------|----------|---------|-------------|
| Ptotal (Mpa)                            | Xi      | Ppartial (Mpa) | Xco2    | KH (Mpa) | ln KH   | 100/T (k-1) |
| 1.20000                                 | 0.97581 | 1.17097        | 0.44444 | 2.63474  | 0.96879 | 0.32987     |

**Table 4.3: Henry's Law Constant at 308.15 K**

| S=700 rpm<br>T= 308.15 K<br>Pi = 21 bar |         |                |         |          |         |             |
|---|---------|----------------|---------|----------|---------|-------------|
| Ptotal (Mpa)                            | Xi      | Ppartial (Mpa) | Xco2    | KH (Mpa) | ln KH   | 100/T (k-1) |
| 1.21000                                 | 0.97562 | 1.18050        | 0.31332 | 3.76771  | 1.32647 | 0.32452     |