Carbon Dioxide Removal by Using Ionic Liquid

by

Irza Bt Hairani

Dissertation submitted in partial fulfilment of
the requirements for the
Bachelor of Engineering (Hons)
(Chemical Engineering)

JANUARY 2009

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CERTIFICATION OF APPROVAL

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Approved by,

(Assoc. Prof Dr. M Azmi b. Bustam)

ABSTRACT

Regarding of many issues faced by the industrial process to remove CO_2. The writer decides to come out with the latest innovation and technology that can overcome the problem. The current technology is using chemical and physical solvent. The major drawback of the traditional gas absorption separation is mainly causes by foaming issues, corrosion issues, effect of impurities and concentration of the solvent. Several issues and challenges that in using current CO_2 removal method is the intensive energy requirements, the corrosivity of the solvents, low CO_2 loading capacity, hazardous to human health and environment, the degradation of amine, and high cost to maintain the solvent. Therefore, new methodology or approach is needed to overcome this problem. The objective of this research was to identify potential Ionic Liquid for CO_2 adsorption and to investigate CO_2 adsorption process by selected Ionic Liquid. There are 3 types of ionic liquid that proved can absorb CO_2 which is 1-*n*-butyl-3-methylimidazolium tetrafluoroborate, $[bmim]^+[BF_4]^-$,1-*n*-butyl-3-methylimidazolium dicyanamide and $[bmim]^+[DCA]^-$ 1-butyl-3-methylimidazolium acetate, $[bmim]^+[acetate]^-$. The criteria considered to chose the ionic liquid is easy to synthesis, have a very low vapour pressure, minimal degradation of ionic liquid, chemically stable, environmentally friendly, have distinct selectivities and having carboxylate moiety bond. However the best among those 3 ionic liquids was chosen due to certain circumstances. In this research it involves several major activities, the preparation of ionic liquid, characterization of ionic liquid, an absorption study on the ionic liquid and result analysis on the ionic liquid. The study also involves a comparison with monodiethanolamine,MEA which is the common chemical solvent that is being used in the process plant. The result from each solvent has been compared in the result analysis. The chosen ionic liquid has proven can absorb CO2 and can be further research for implementation in the process industry.

ACKNOWLEDGEMENTS

The author wishes to take the opportunity to express her utmost gratitude to the individual that have taken the time and effort to assist the author in completing the project. Without the cooperation of these individuals, no doubt the author would have faced some minor complications through out the course.

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For all the team in Ionic Liquid lab, the Research Officer, Mrs Naim, Miss Mona, Miss Hawa, and Miss Hasiah for helping the author regarding the lab work.

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CHAPTER 1

INTRODUCTION

1.1 Introduction

Chemical and physical absorption processes are extensively used in natural gas, petroleum, and chemical industries for the separation of CO_2. Aqueous solutions of Diethanolamine are one of the solvents used for CO_2 removal. One of the common solvents used is Benfield solution from UOP the licensee of this solvent. The Benfield solution consists of

i. Potassium Carbonate (K_2CO_3)
ii. Diethanolamine (DEA)
iii. Vanadium Pentaoxide (V_2O_5)
iv. Demineralised water as base solution

Reaction mechanism to absorb CO_2 is

$$K_2CO_3 + CO_2 + H_2O \rightarrow 2KHCO_3 + \text{Heat}$$

Then to recover the K_2CO_3 solution, the reaction mechanism is:

$$2KHCO_3 + \text{Heat} \rightarrow K_2CO_3 + CO_2 + H_2O$$

Diethanolamine in this solution acts as the catalyst while Vanadium Pentaoxide acts as the corrosion inhibitor.

About 90 to 98% of the CO_2 in the natural gas will be absorbed by using this solvent. However, as the solution being regenerate the CO_2 loading capacity in the Benfield solution decreases. Therefore, there are strong incentives for the development of low cost and efficient alternatives.

The major drawbacks of the traditional gas absorption separation are mainly causes by these issues:

a) Foaming issues
b) Corrosion issues
c) Effect of impurities
d) Concentration of solvent

Besides that, current research on the system also showed that there are some problem regarding the higher CO_2 slippage from the process. It can be due to the following reasons:

- Amount of CO_2 to the absorber versus the absorbing capacity
- Lean solution circulation rate
- Solution composition such as the concentration of K_2CO_3
- Absorber and regeneration operating parameters

In an industrial gas absorption process it is desirable to achieve fast absorption rates and high solute capacity into a solvent that is easily regenerated and volume make-up is minimized.

In the search of alternative liquid phase absorbent for CO_2 capture technology, scientists found that room temperature ionic liquid can be expected as good alternative candidates to replace already established amine-based solution, such as MEA, MDEA or piperazine for CO_2 absorption. Although amine-based scrubber is very effective in adsorbing CO_2 through a chemical interaction and an intermediate carbamate formation, its application in industrial scale still faces some problems mainly the corrosion due to the strong basic property, the low thermal stability and the high energy demand for CO_2 desorption process. In that regard, a highly effective CO_2 physical adsorption should be introduced as an alternative CO_2 adsorption process.

Carbon Dioxide is undesired components that are found in many natural gas and other gas sources. The removal of CO_2 is required to improve the fuel quality (heating value) of the natural gas. Besides that, CO_2 in the presence of water can be a corrosive agent to metal pipes. The need to remove CO_2 from gas stream in a gas processing plant is crucial to prevent corrosion and dry ice formation in the low temperature chillers. In our gas plant, we use chemical solvents to absorb CO_2 form the natural gas. However, we have to face several issues and challenges in using the chemical solvents, these are the issues:

i. Intensive energy requirements- Throughout the regeneration step, heating energy is required to break the chemical bonds between the absorbed CO_2 and solvent. This energy requirement can be very high and represents significant operating expenses in the plant.

ii. Corrosivity of the amine- the amine solution is corrosive to low alloy steel such as carbon steel. In order to prevent the corrosion, other chemical such as corrosion inhibitor, Vanadium Pentaoxide is needed in the solution.

iii. CO_2 loading capacity- CO_2 loading capacity is limited by the concentration of the amine solution

iv. The solution is hazardous to human and environment.

v. Degradation of amine

vi. High cost to maintain the chemical

Ionic liquids have been used as reaction media, in separation and extraction processes and furthermore, these seem suitable for being use as a solvent in gas absorption. Ionic liquids are new and exciting class of compound that have the potential to overcome many of the problems associated with current CO_2 capture techniques. Ionic liquids (ILs) are organic salts that are in their pure state near ambient conditions. ILs are regarded as potentially environmentally-benign solvents due to their immeasurably low vapor pressure, which essentially eliminates the opportunity for solvent release to the atmosphere.

1.2 Problem Statement

Regarding the problems that have been faced by physical and chemical solvent, it is crucial to find alternative technology to remove CO_2. However, the current research on CO_2 absorption on ionic liquid is not adequate.

1.3 Objectives

1. To identify potential ionic liquid for Carbon Dioxide adsorption
2. To investigate Carbon Dioxide adsorption process by selected ionic liquid

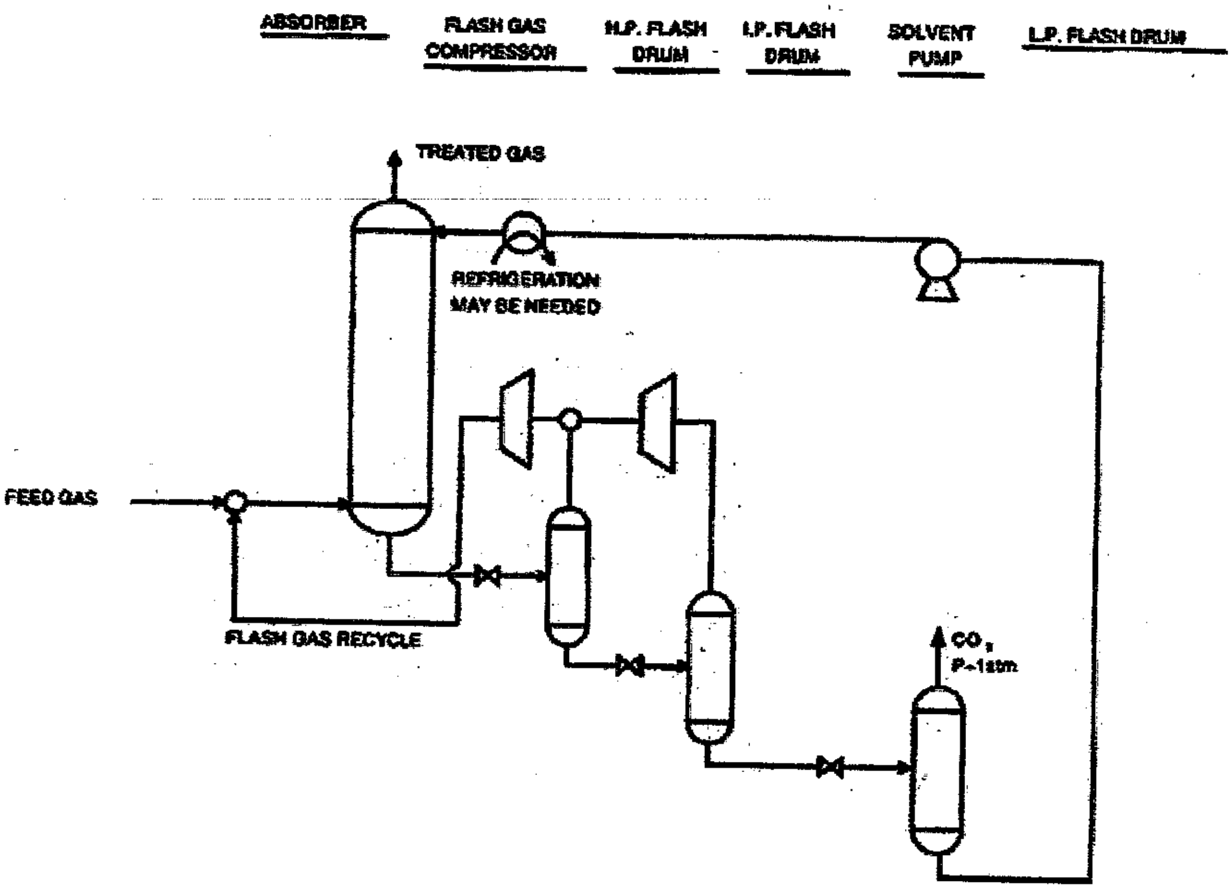


Figure 1: Simple process flow diagram for physical absorption process

1.4 Scope of work

For this project the scope of work will be focused on three activities:

a) Synthesis

- After the research is done and the suitable ionic liquid has been chosen, the preparation for the Ionic Liquid should be done. Every Ionic Liquid have their own way to synthesized.

b) Physical property measurement

- Once the Ionic Liquid have been prepared, conduct several test on the Ionic Liquid to determine the properties and the characteristics of the Ionic Liquid.

c) Experiment

- Finish with the synthesizing, the absorption study on CO_2 should be carried out. In this experiment, the effectiveness and the suitability of the chosen Ionic Liquid could been proved or otherwise.

d) Result Analysis

- After the experiment, an analysis on the result sample should be conducted using FTIR and TGA equipment.

CHAPTER 2

LITERATURE REVIEW

2.1 Background Studies

Since their emergence a decade ago, ionic liquids (IL) have had a constantly growing influence on organic, bio- and green chemistry, due to the unique physico-chemical properties manifested by their typical salt structure: a heterocyclic nitrogen-containing organic cation (in general) and an inorganic or organic anion, with melting points below 100 °C and no vapor pressure. The latter property leads to the practical replacement of conventional volatile organic compounds (VOCs) from the point of view of atmospheric emissions, though they do present the serious drawback that a small amount of IL could enter the environment through groundwater. This risk makes it necessary to perform further eco-toxicological studies of IL on various species, in order to improve the "design rules" for synthesized IL with minimal toxicity to environment integrated organisms.

Ionic liquids display variable stability in terms of moisture and solubility in water, polar and nonpolar organic solvents. Various values of ionic liquid hydrophobicity and polarity may be tailored with the help of nucleoside chemistry according to the main principles of green chemistry: the new chemicals must be designed to preserve effectiveness of function while reducing toxicity, and not persisting in the environment at the end of their usage, but breaking down into inoffensive degradation products. Most of the ionic liquids with imidazolium, phosphonium, pyridinium and ammonium that were tested were resistant to ready biodegradation. Their toxicity to microorganisms can limit biodegradation, while their toxicity to humans and others organisms is obviously significant.

The examination regarding the biodegradation of surfactant compounds focuses on a close resemblance between many quaternary ammonium compounds as well as surfactants based around an imidazolium core. The factors that improved the biodegradation of surfactants have successfully been applied to ionic liquids. The enzymatic hydrolysis step, which initiates a pathway to further breakdown products, improves the biodegradation. Therefore, compound stability and toxicity are the factors biodegradability depends on. The effect of the counter-ion was not noticeable in biodegradability even though modifications of the anion led to changes in physical and chemical properties. Still, the introduction of an organic anion clearly improves the extent of ultimate biodegradation

From the point of view of reactivity, IL generally do not coordinate to metal complexes, enzymes and different organic substrates; however, they are usually the major component of the mixtures having pre-organized structures with the aid of many hydrogen bonds (structural directionality) in contrast to classical salts in which the compounds are mostly formed with the aid of ionic bonds (charge-ordering structures). On the other way, the recycling ability of IL, especially dialkyl-imidazolium based ionic liquids (the most studied until now), is based on their lack of solubility in some key organic solvents. Water/soluble ionic liquids are more difficult to recycle, since their water immiscible complements, the secondary products, cannot be easily removed.

Ionic Liquid are known as a new, unique and exciting class of solvents that cold potentially replace volatile organic solvents currently being used in large volume. They are composed of a bulky and organic cation as well as organic or inorganic anions and are liquid at room temperature, mainly due to the large asymmetrical cations preventing close packing of the ions, which can cause their low melting points. Since the melting points are low, ionic liquids can act as solvents in which reaction can be performed, and because the liquid is made of ions rather than molecules, such reactions often give distinctive selectivities and reactivity when compared with conventional organic solvents.

Ionic liquids have no significant vapour pressure and thus create no volatile organic compounds. They also allow for easy separation of organic molecules by direct distillation without loss of the ionic liquid. The nature of the cation and the anion determines the physical and chemical properties of the ionic liquid. Therefore, it is possible to achieve specific properties by choosing the proper combination of a cation and anion as effect of the existing dependence between the properties and the constituent ions of ionic liquids.

Ionic liquid are generally non-volatile, with effectively no vapor pressure. Many are air and water stable, and can be good solvents for a wide variety of inorganic, organic and polymeric materials. The properties of ionic liquids can be tailored by varying the cation and anion pairing. Ionic Liquid is attracting increasing attention from industry because they promise significant environmental as well as products and process benefits. The advantages for Ionic liquid are summarized in the table below:

Properties	**Remarks**
Low melting points	IL can react as solvents where reactions can be performed
Made of ions	Give distinctive selectivities and reactivity
No vapour pressure	No volatile organic compounds, easy separation of organic compounds
Good solvents	Allow small reactor to be utilised
High thermal stability	Reaction may be carried stably and easily separated from the reaction product
Non-flammable	Low combustibility
Wide liquid range	Allowing for large reaction kinetic control

Table 1: Properties of Ionic Liquids

Development of alternatives for innovative chemical technologies, which introduce widely used chemicals in industry in order to reduce the use or generation of hazardous substances, eliminate corrosion problems, and lower energy consumption has always been of particular interest. Some of the features of ionic liquids such as their application as environmentally safe, non-corrosive media for absorption of acidic gases in the process of natural gas refining, where they replace amines and thereby increase production capacities of gas refineries. Furthermore, obtaining expensive and higher purity grade chemical and petrochemical products using Ionic Liquid can be of great importance.

Many ionic liquids are formed by reacting a nitrogen-containing heterocyclic ring, preferably a heteroaromatic ring, with an alkylating agent to form a quaternary ammonium salt, and performing ion exchange or other suitable reactions with various Lewis acids or their conjugate bases to form ionic liquids. These rings can be alkylated with virtually any straight, branched or cyclic C_{1-20} alkyl group, but preferably the alkyl groups are C_{1-12} groups, since groups larger than this tend to produce low melting solids than ionic liquids.

In order to fulfill the objectives, search for the IL with following characteristics:

a) Absorbs high amounts (per mass) of CO_2
b) Selective towards CO_2 and does not absorb O_2, N_2, water or other gases.
c) Absorbs reversibly so the CO_2 can be taken out easily
d) Reusable
e) Cheap
f) Low viscosity for easier use in industrial facilities
g) Can be synthesized with low waste production and low energy consumption

To screen the appropriate IL based CO_2 adsorption system, solubility measurement is essential to carry out. Various techniques have been introduced which fall into three different types:

i. Gravimetric method using microbalance
ii. Isochoric method based on pressure drop
iii. Transient thin-liquid-film method

CHAPTER 3

METHODOLOGY

Based on the scope of work before, there are three activities that should be focused on:

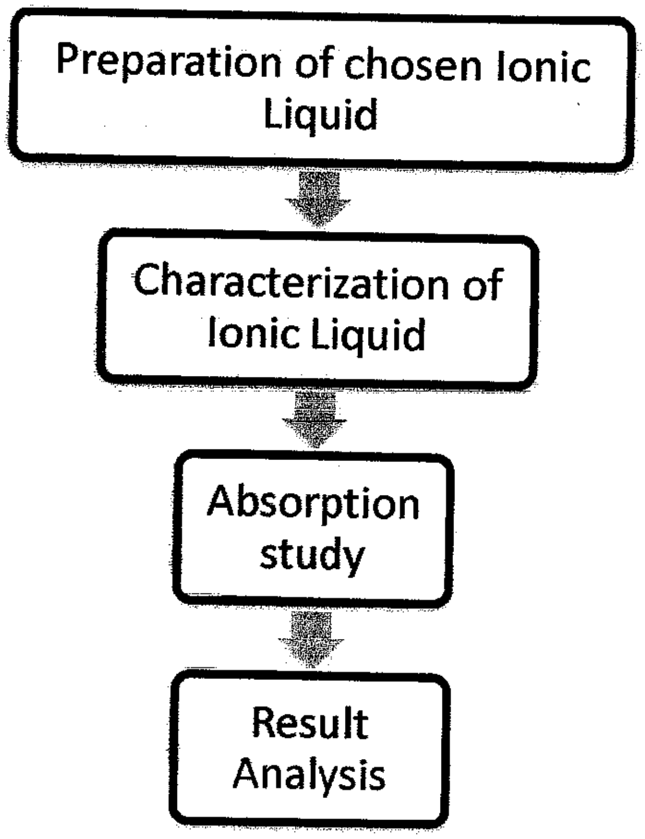


Figure 2: Methodology

Before we could start with the absorption study, we should do the preparation for the chosen Ionic Liquid. The synthesis of Ionic Liquid is different depends on the Ionic Liquid needed. After the preparation of the Ionic Liquid, the Ionic Liquid properties and charaterisation should be determined. From the test we could determined on the end result after the absorption study. Then, the absorption study should be conducted. In this study, the CO_2 gas will be flowed into the Ionic Liquid. After that, the characterization and properties test of Ionic Liquid will be conducted to determine the effect of CO_2 absorption to the IL.

3.1 Preparation of Ionic Liquid

A wide research is conducted in order to determine the best Ionic Liquid that can be used in CO_2 removal system. From the research, there are 3 Ionic Liquids that have been proved can absorb CO_2.

i. 1-*n*-butyl-3-methylimidazolium tetrafluoroborate, $[bmim]^+[BF_4]^-$

1-Butyl-3-methylimidazolium **Tetrafluoroborate**

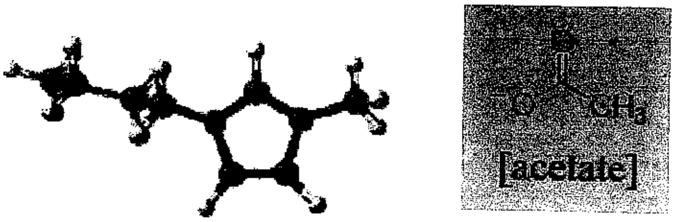
Figure 3: 1-butyl-3-methylimidazolium tetrafluoroborate

ii. 1-*n*-butyl-3-methylimidazolium dicyanamide, $[bmim]^+[DCA]^-$

1-Butyl-3-methylimidazolium **Dicyanamide**

Figure 4: 1-butyl-3-methylimidazolium dicyanamide

iii. 1-butyl-3-methylimidazolium acetate, $[bmim]^+[acetate]^-$



1-Butyl-3-methylimidazolium

Figure 5: 1-butyl-3-methylimidazolium acetate

Due to unavailability of some of the solvent, the Ionic Liquid chosen is 1-butyl-3-methylimidazolium tetrafluoroborate

Chosen Ionic Liquid

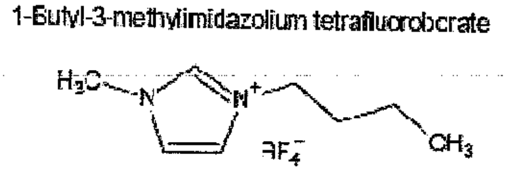


Figure 6: 1-Butyl-3-methylimidazolium tetrafluoroborate

Chemical Name: 1-Butyl-3-methylimidazolium tetrafluoroborate
Chemical Formula: $C_8H_{15}N_2.BF_4$
Molecular Weight: 226.02
Density: 1.2077
Appearance: Clear, Colourless viscous liquid

It has been discovered that absorbents containing an ionic liquid having an anion comprising a carboxylate moiety have a particularly useful set of features for separation and or removal of CO_2 from a gaseous stream. The suitable Ionic Liquid for CO_2 removal is 1-butyl-3-methylimidazolium (bmim) tetrafluoroborate. This ionic liquid is known as environmentally friendly and recyclable solvents. It is also moisture stable but water miscible. It is depend on the ratio of ionic liquid to water, system temperature and alkyl chain length in the cation.

The advantages of choosing this type of ionic liquid is that its have a very low (effectively zero) vapor pressure, so potential for IL absorbent being lost in the gaseous product is minimal. Besides that, the carboxylate moiety interacts with water to form a weak reversible bond with CO_2. This type of ionic liquid also is chemically stable and has a minimal degradation. For the cation, the CO_2 solubility increases with increasing chain length.

The reason why do we choose this ionic liquid was because:

i. Easy to synthesis - easier to maintain the solvent in the gas processing plant
ii. Have very low vapor pressure – potential for the IL absorbents to be lost is minimal
iii. The solvent has a minimal degradation – no need to recover the solution
iv. Chemically stable
v. Environmentally friendly – not hazardous to human health and environment
vi. Have distinct selectivities
vii. Carboxylate moiety bond- form a weak reversible bond with CO_2 therefore it only required lower heating energy to break the bond

3.2 Characterization of Ionic Liquid

There are 3 methods that can be used to determine the characteristics of ionic liquid

i. Thermogravimetric Analysis
   - Thermogravimetric Analysis is a type of testing that is performed on samples to determine changes in weight in relation to change in temperature.
   - This analysis relies on a high degree of precision in three measurements: weight, temperature, and temperature change.
   - TGA is commonly employed in research and testing to determine the characteristics of material, to determine degradation temperatures, absorbed moisture content of materials, decomposition points of explosives, and solve residues.

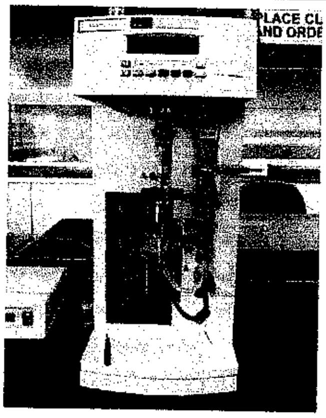


Figure 7: Thermogravimetric Analyzer

ii. Fourier Transform Infrared Spectrometry
   - This equipment is a measurement technique whereby spectra are collected based on measurements of the temporal coherence of a radiative source. It will provide the quality or the consistency of a sample, the amounts of components in a mixture and the identity of unknown materials.
   - For Ionic Liquid, the analysis have to use Demountable Liquid Cell form ZnSe Window (32x3mm drilled) and ZnSe Window(32x3mm) from PIKE Technologies.

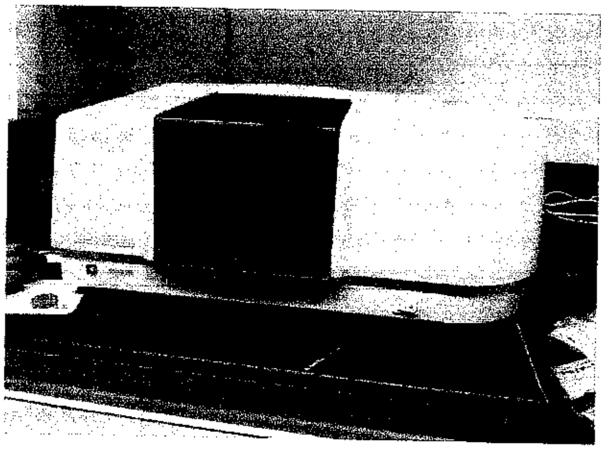


Figure 8: FTIR equipment

iii. **Ultraviolet-Visible Spectroscopy (UV-Vis)**

- UV-Vis involves the spectroscopy of photons in the UV-visible region. It is used in the quantitative determination of solutions of transition metal ions and highly conjugated organic compounds. It can measure the concentration of an analyte in solution by measuring the absorbance at some wavelength and applying the Beer-Lambert law.

The analysis on the solvent will undergo two tests in FTIR and TGA in order to determine the purity and composition in the solvent before the experiment. The analyse will repeated after the experiment has been conducted.

3.3 CO2 Absorption Study

Experimental work:

Carbon Dioxide Removal using 1-butyl-3-methylimidazolium tetrafluoroborate

Objective

To discover the solubility of Carbon Dioxide in Ionic Liquid

Sample Test:

Before doing the experiment, conduct several tests on the ionic liquid:

1. FTIR (IR Analyzer)
2. TGA

Chemicals:

1. 1-butyl-3-methylimidazolium tetrafluoroborate, [bmim][BF4]
2. Pure Carbon Dioxide

Apparatus:

1. 120mL plastic beaker
2. Gas Tube

Method:

1. Prepare the purified CO2
2. Put 30mL of [bmim][BF4] into a closed vessel at room temperature and pressure
3. Flow the natural gas from the bottom of the closed vessel
4. Let the flow of gas for 60 minutes
5. Run a FTIR test on the sample

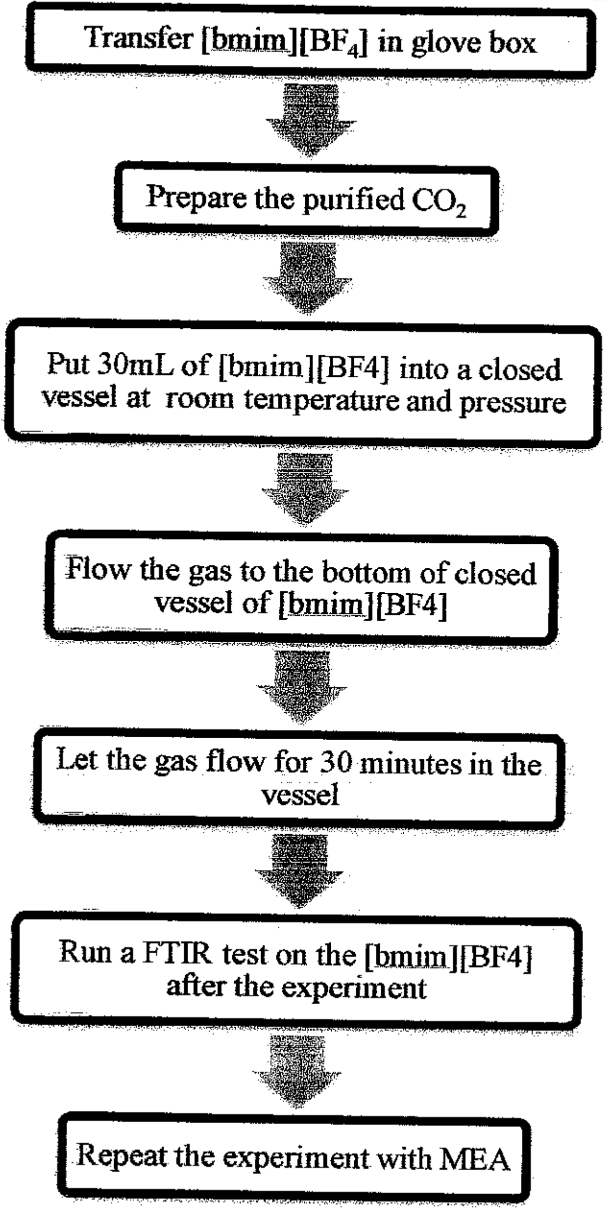


Figure 9: Methodology for absorption study

This experiment will repeated by using Monoethanolamine (MEA). By this way, the absorption rate for each solvent will be determined.

Solvents used in this experiment is:

i. 1-*n*-butyl-3-methylimidazolium tetrafluoroborate, $[\text{bmim}]^+[\text{BF}_4]^-$

  - This Ionic Liquid is chosen due to its very low (effectively zero) vapor pressure. So the potential for IL absorbent being lost in the gaseous product is minimal. This ionic liquid is known as environmentally friendly and recyclable solvents. This type of ionic liquid also is chemically stable and has a minimal degradation.

ii. Monoethanolamine

  - A chemical intermediate in the manufacture of cosmetics, surface-active agents, emulsifiers, pharmaceuticals, and plasticizing agents; a gas-scrubbing agent for the absorption and removal of H_2S and CO_2 from refinery and natural gas streams; carbon dioxide and ammonia manufacturing.
  - This chemical solvent is established for a long time as a CO2 removal. This type of solvent is commonly used in process plant industry.

3.4 Observation from the experiment

i. On [bmim][BF4]

- During the experiment, the Ionic Liquid did not show any changes on color or in the temperature. However, we can see that bubbles formed in the vessel after the experiment. Below is the reaction mechanism between [bmim][BF4] and CO2[1].

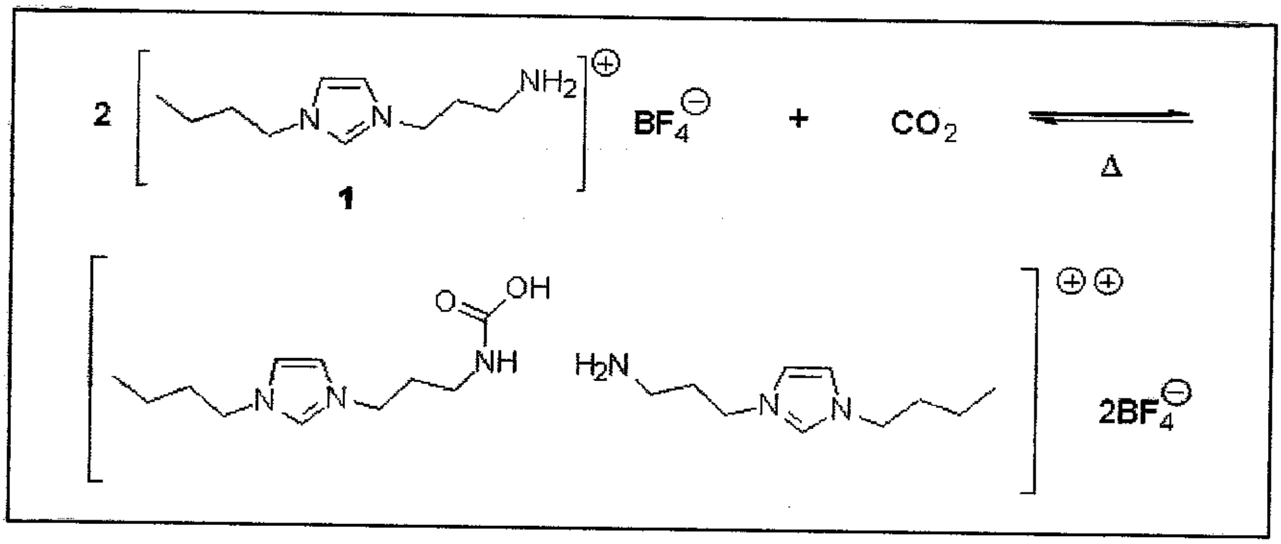


Figure 10: Reaction mechanism in [bmim][BF4]

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[1] CO2 capture by a task specific Ionic Liquid, Eleanor D. Bates, Rebecca D. Mayton, Ioanna Ntai, and James H. Davis, Jr.

ii. On Monoethanolamine,MEA

- When MEA is being exposed to the Carbon Dioxide the temperature of the sample increases. The reaction between the MEA and Carbon Dioxide releases heat. Besides that, after being exposed to CO2, the MEA become more viscous compared before.
- The reaction mechanism for Monoethanolamine with CO2 is

$$C_2H_7NO + H_2O + CO_2 \text{ J } H_3O^+ + C_3H_6NO_3$$ [2]

Figure 11: Sample of MEA

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[2] Carbon Dioxide Removal, Alex Bubulka, Breanna Kelly

CHAPTER 4

RESULT & DISCUSSION

In order to determine the composition in the solvents after the experiment, a result analysis is conducted on the sample. The analysis is done by Fourier Transform Infrared (FTIR) equipment. The main goal of IR spectroscopic analysis is to determine the chemical functional groups in the sample. Different functional groups absorb characteristic frequencies of IR radiation.

4.1 Characteristics of [bmim][BF4]

4.1.1 FTIR Analysis

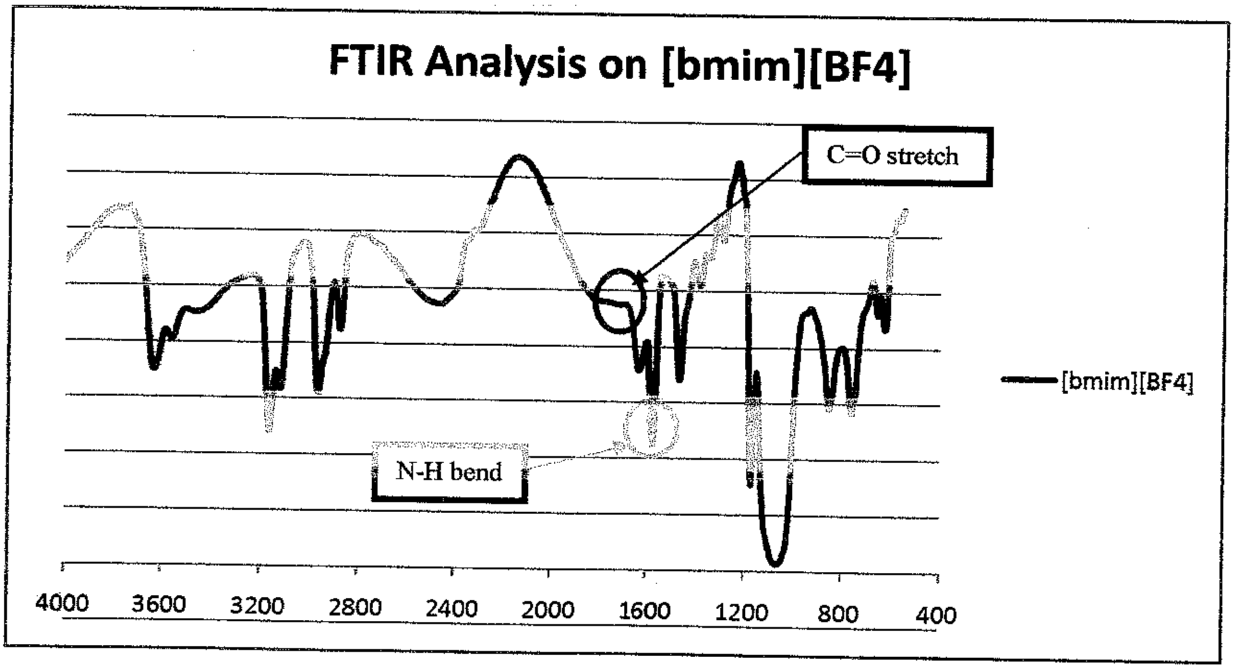

Figure 12: Characterization of Ionic Liquid

Based on the FTIR result, the characterics of [bmim][BF4] can be determined by interpreting the peaks in the result. At 1680-1630 cm^{-1}, the C=O stretch is not visible yet before the sample exposed to the Carbon Dioxide. The important component in [bmim][BF4] is the N-H bend as the C=O bond will attack this bend in the reaction later. The N-H bend is located at 1640-1500 cm^{-1}.

4.1.2 TGA Analysis

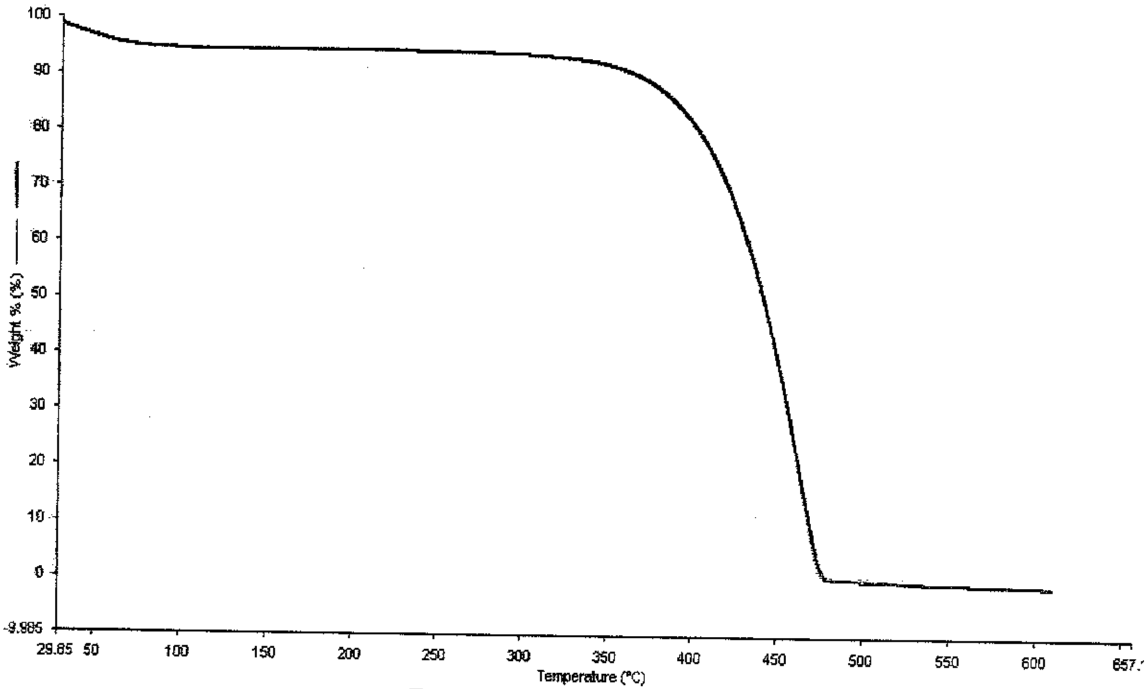

Figure 13: TGA Analysis

TGA analysis is conducted to prove that the ionic liquid is chemically stable and can withstand high temperature. From the analysis, the decomposition of ionic liquid only started after 400°C. Therefore, it proves that this ionic liquid is chemically stable and can withstand high temperature.

4.2 Results on [bmim][BF4]

An analysis was conducted on the sample after the experiment. The composition in the sample is based on the infrared spectroscopy. Check the wavenumber in the FTIR analysis and determine its molecular motion in the infrared spectroscopy table. Below is the basic peaks for the analysis.

BASIC PEAKS	
Molecular Motion	Wavenumber (cm-1)
CH2 bend	~1465
C=C stretch (isolated)	1690 - 1630
C-H bend (mono)	770-730 & 715-685
C-H bend (para)	850-800
O-H stretch	~3650 or 3400-3300
C=O stretch	1680-1630
N-H bend	1640-1500
C-O-C stretch	1300 – 1000

Table 2: Basic Peaks of Wavelength

i. Comparison on [bmim][BF4] before and after absorption study

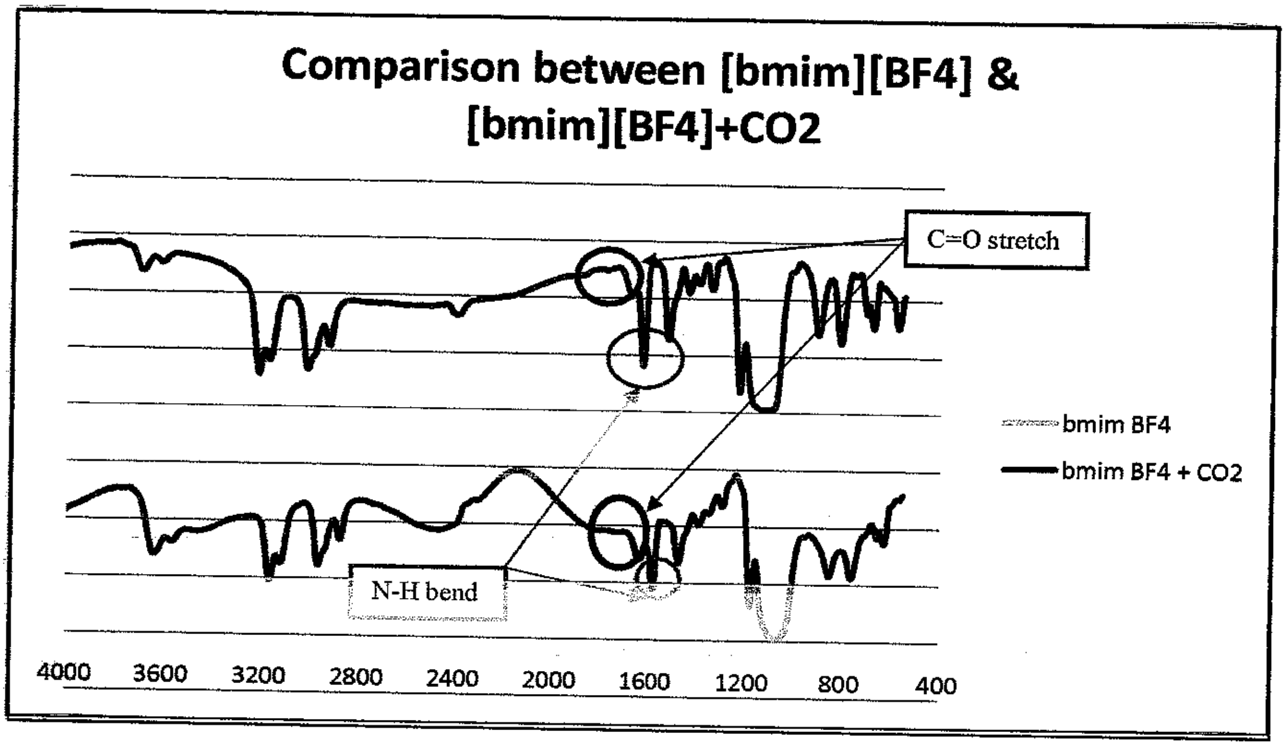

Figure 14: FTIR Analysis [bmim][BF4]

From the FTIR analysis, before we can see some differences in the peak. At wavelength of 1680-1630 cm^{-1}, we can see the C=O stretch has formed. The peak is visible after the ionic liquid has been exposed to the CO2. At wavelength of 1640-1500 cm^{-1}, the peak for N-H bend is increased because the N-H bond has been break in the absorption process.

4.3 Results on Monoethanolamine, MEA

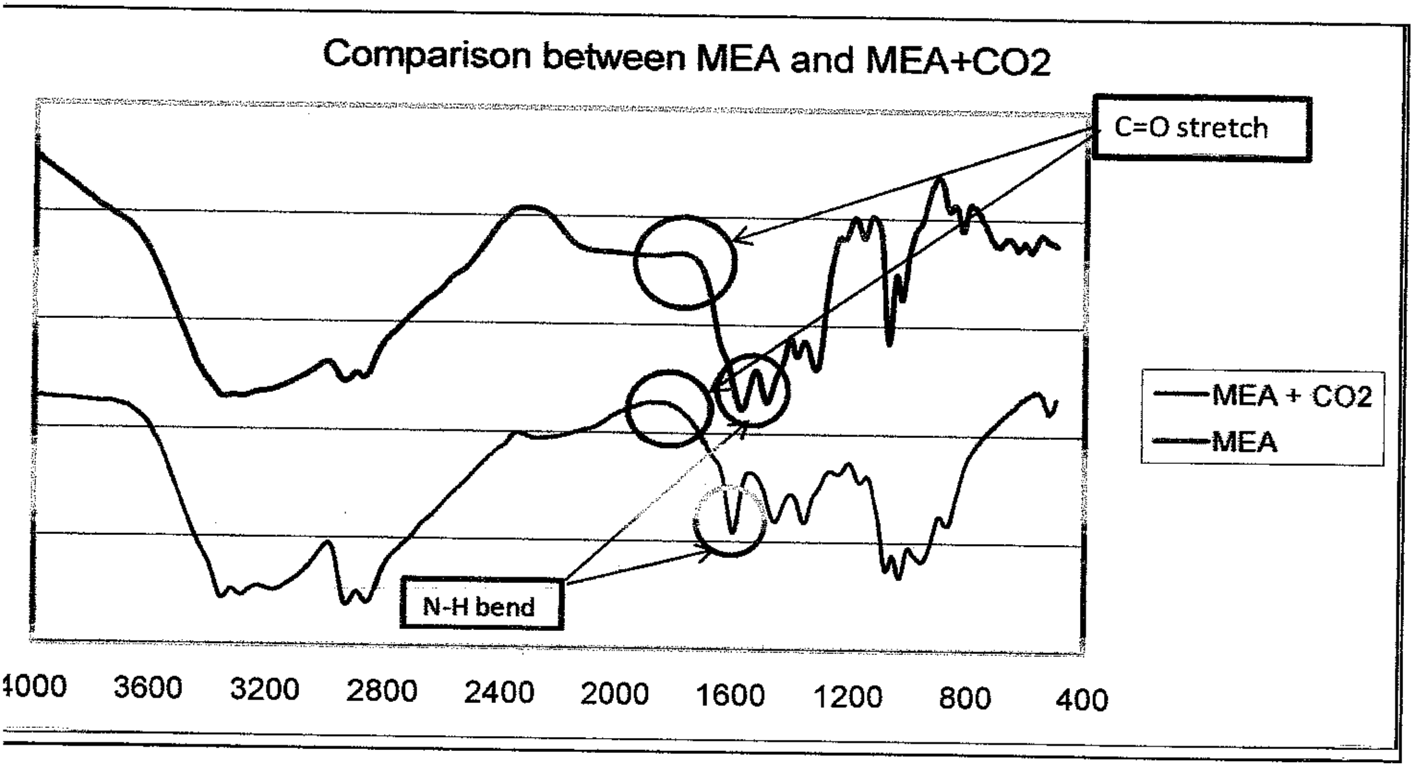

Figure 15: FTIR Analysis on MEA

Compare the monoethanolamine before the experiment and after the experiment. After being exposed to CO2 the C=O stretch become visible. It shows that the MEA has already absorbed the CO2. The peaks for C=O stretch is also forms at 1680-1630 cm^{-1} after the experiment. The N-H bend at 1640 – 1500 cm^{-1} was increased after the absorption study indicates that NH component in the MEA increased after the experiment

CHAPTER 5

ENVIRONMENTAL IMPACT

One of the main concerns on Benfield solution is the heavy metal that contains in it which is the Vanadium Pentaoxide that is hazardous to human health and environment. In other hand, the Ionic Liquid are frequently referred to as 'environmentally benign' due to their immeasurably low vapour pressure. In this respect, ionic liquids have emerged as a set of green solvents with unique properties such as tunable polarity, high thermal stability and immiscibility with a number of organic solvents, negligible vapor pressure and recyclability. Their high polarity and the ability to solubilize both organic and inorganic compounds can result in enhanced rates of chemical processes and can provide higher selectivities compared to conventional solvents. Because of distinct advantages of ionic liquids as environmentally benign reaction media for catalytic processes, much attention has currently focused on organic reactions promoted by ionic liquids.IL are environmentally-friendly alternatives to organic solvents for liquid/liquid extractions, catalysis, separations, and electrochemistry. IL will reduce or eliminate the related costs, disposal requirements, and hazards associated with volatile organic compounds (VOCs). The ability to fine-tune the properties of the IL medium will allow selection of IL to replace specific solvents in a variety of different processes.

Due to their non-volatility, effectively eliminating a major pathway for environmental release and contamination, ionic liquids have been considered as having a low impact on the environment and human health, and thus recognized as solvents for green chemistry. Green chemistry is the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances. However, this is distinct from toxicity, and it remains to be seen how 'environmentally-friendly' ILs will be regarded once widely used by industry. Research into IL aquatic toxicity has shown them to be as toxic as or more so than many current solvents already in use.

Being a non-toxic solvent, the ionic liquid can make its way to replace the use of chemical solvents that contains heavy metal in the future.

CHAPTER 6

CONCLUSION

6.1 Conclusion.

The objective to prove that Ionic Liquid can be used to remove CO_2 has been accomplished. By implementing this new method in the Acid Gas Removal Unit to remove CO_2, the energy requirements could be reduced. In other hand, Ionic Liquid is also an environmental friendly chemicals and non-hazardous to human health and to the environment. By comparing the Ionic Liquid to MEA has proved that the Ionic Liquid is capable to replace the usage of MEA in process plant in the future.

It can be concluded that the Ionic Liquid is capable as the solvent media in CO_2 removal in the future. The implementation of this chemical in a process plant is possible after a few more research.

6.2 Recommendation.

Several things can be done in order to improve the project:

- Make sure all the equipment is well calibrated and maintenances are done frequently. Therefore errors could be avoided.
- Further research on the operating conditions of the sample.

REFERENCE

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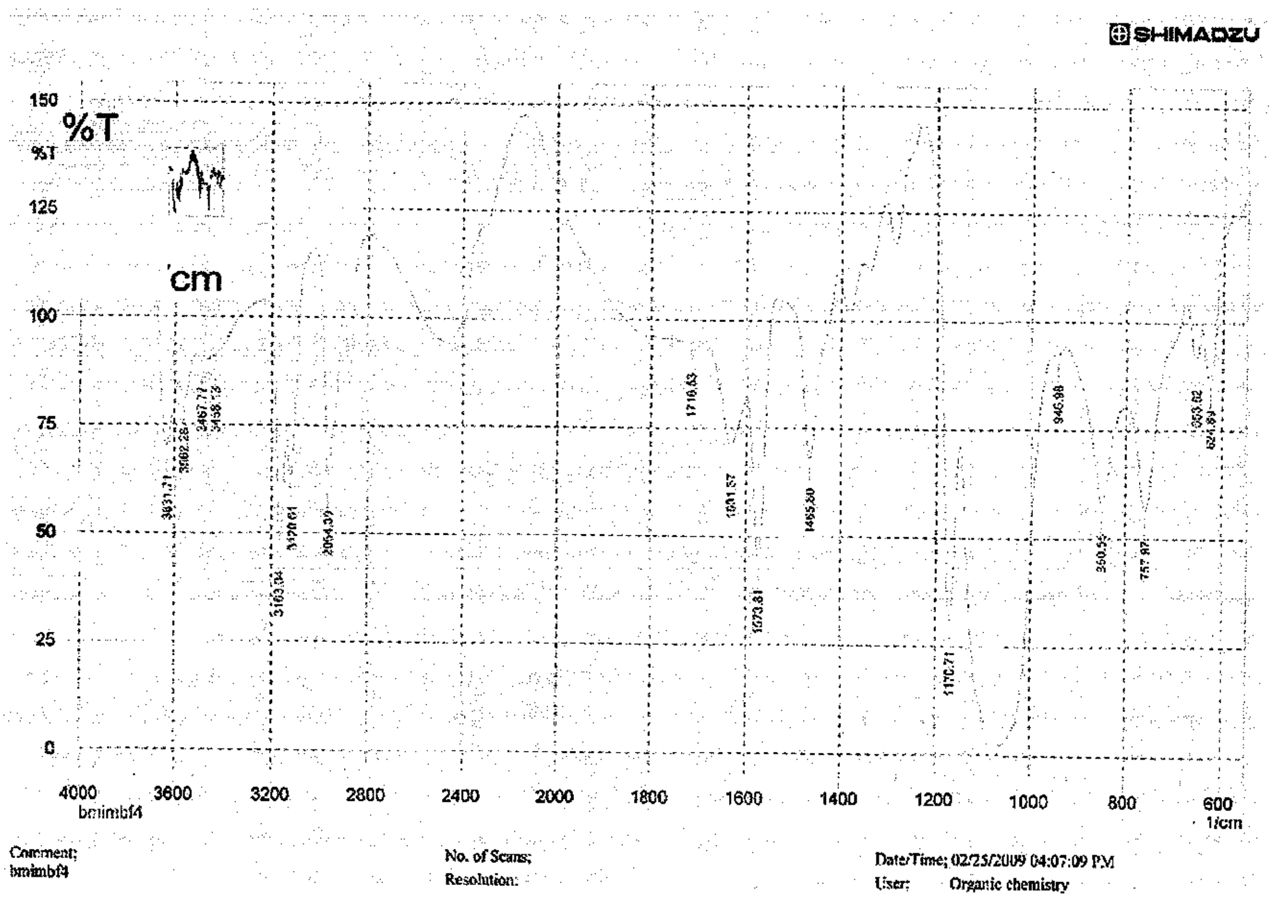
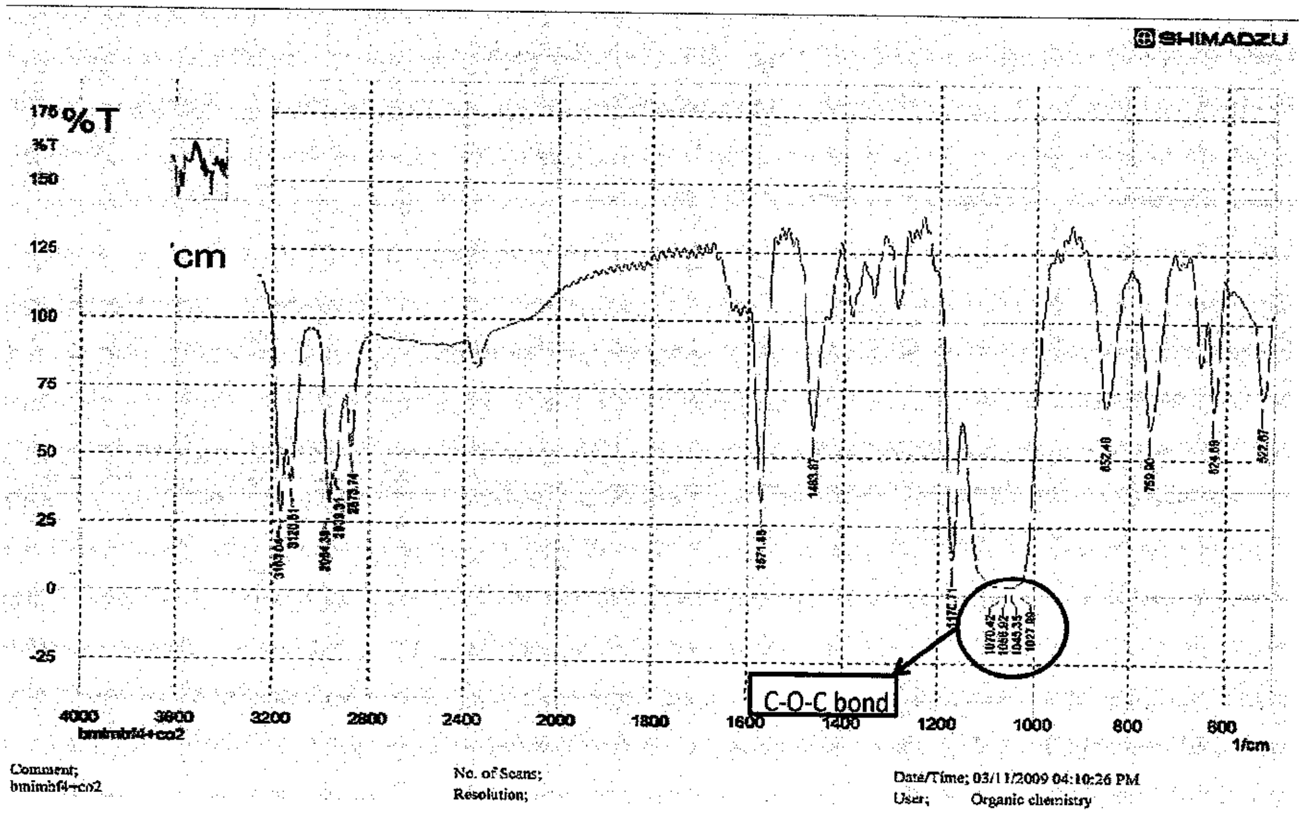
APPENDIX

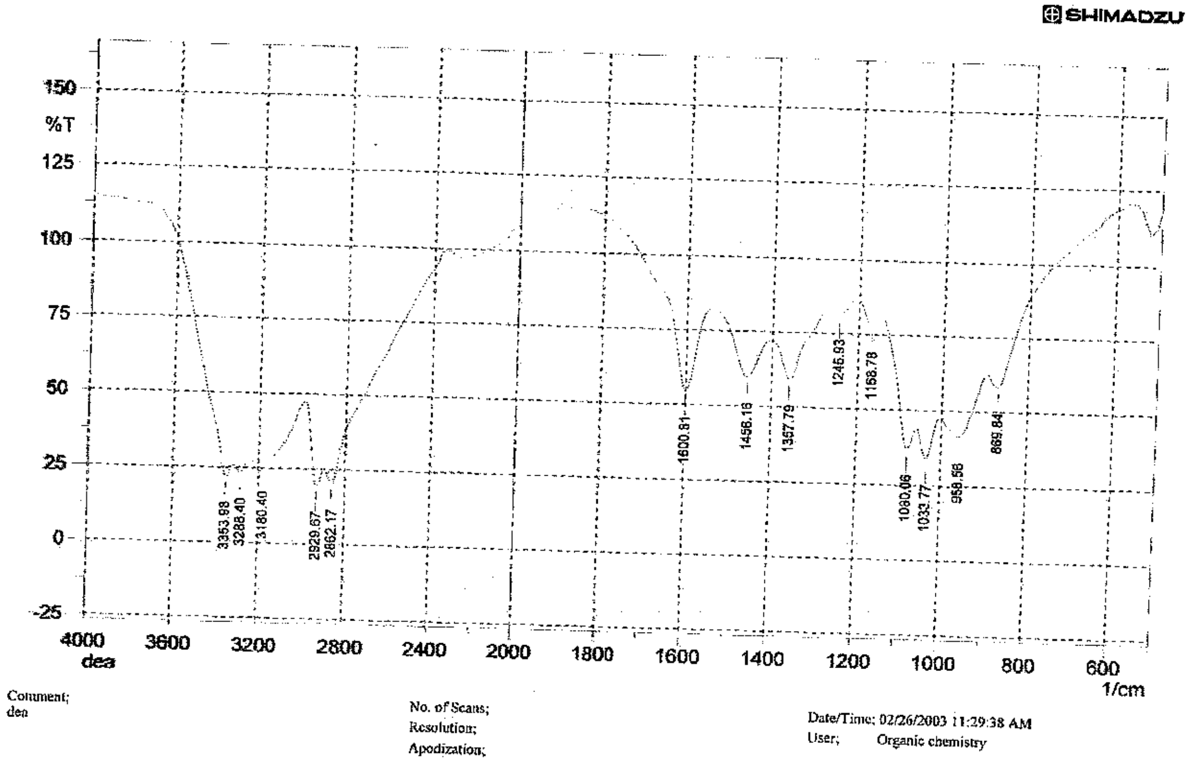
Appendix A : Raw Data of FTIR Analysis on [bmim][BF4]



Appendix B: Raw Data of FTIR Analysis on [bmim][BF4] + [CO2]



Appendix C: Raw Data of FTIR Analysis on MEA

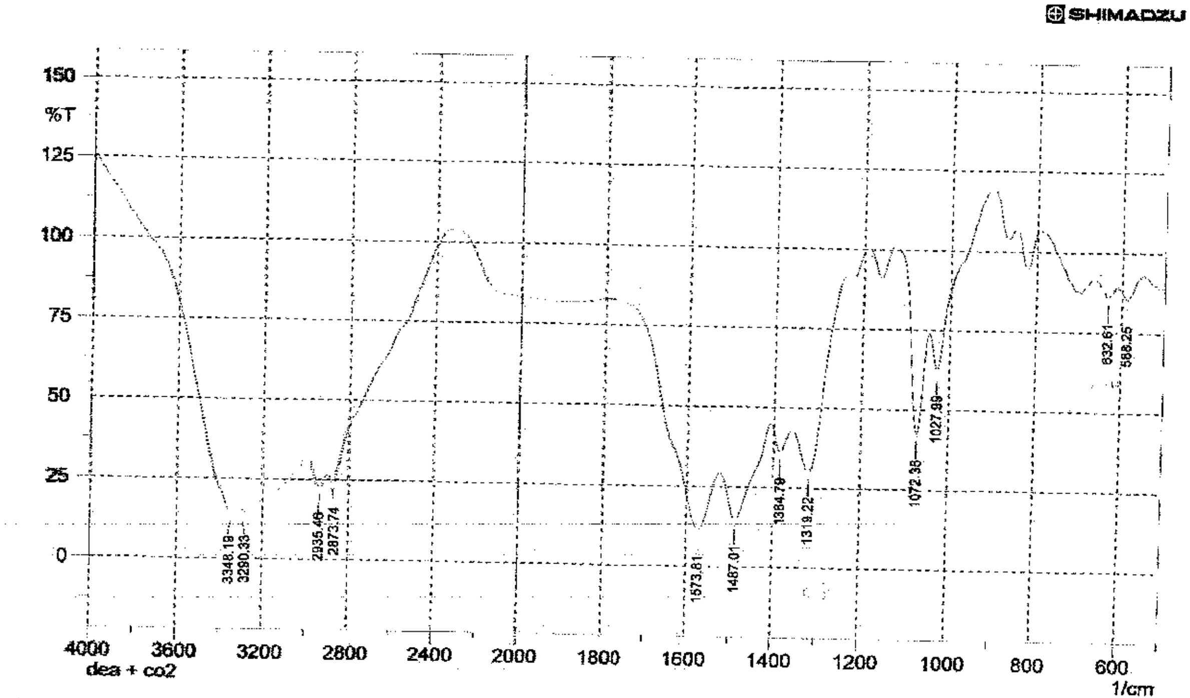


Comment;
dea

No. of Scans;
Resolution;
Apodization;

Date/Time; 02/26/2003 11:29:38 AM
User; Organic chemistry

Appendix D: Raw Data of FTIR Analysis on MEA + CO2



Comment;
dea + co2

No. of Scans;
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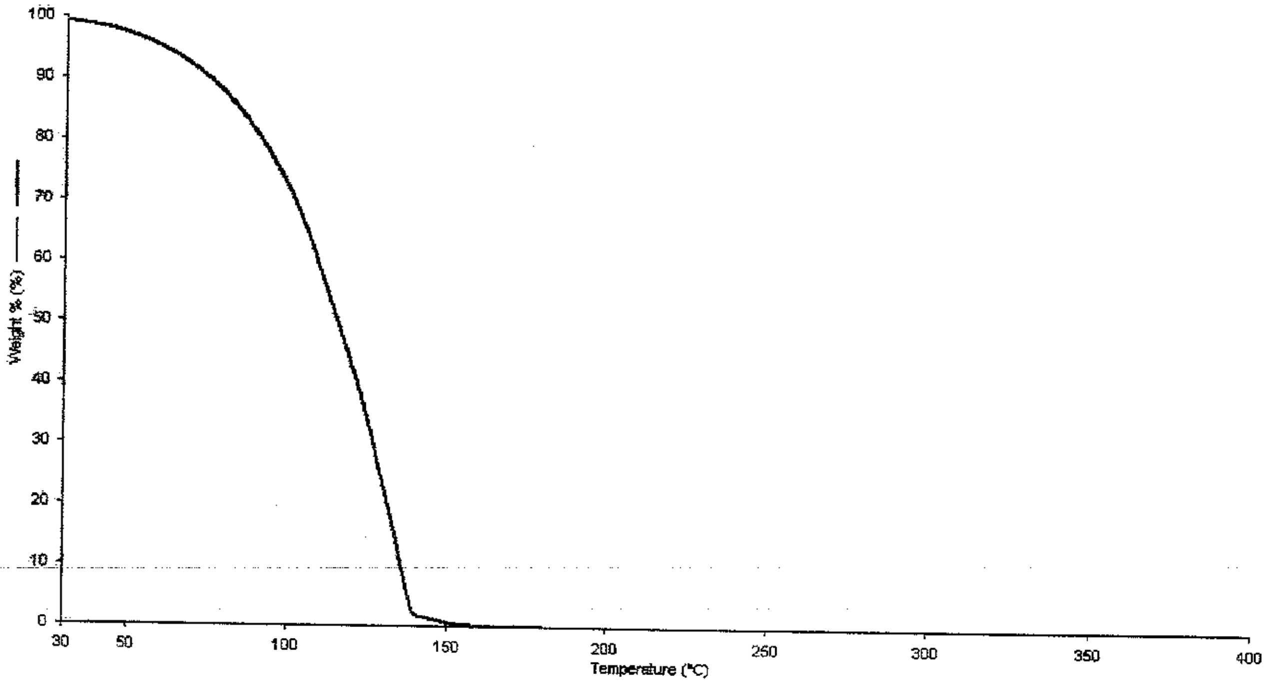
User; Organic chemistry

APPENDIX E : TGA Analysis on MEA



APPENDIX

F

[MSDS]

MERCK

Safety Data Sheet

According to EC Directive 91/155/EEC

Date of issue:	23.02.2005
Supersedes edition of	27.07.2004

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1. Identification of the substance/preparation and of the company/undertaking

Identification of the product

Catalogue No.:	491049
Product name:	1-Butyl-3-methylimidazolium tetrafluoroborate high purity

Use of the substance/preparation

Reagent for development and research
Solvent
Chemical for synthesis

Company/undertaking identification

Company:	Merck KGaA * 64271 Darmstadt * Germany * Phone: +49 6151 72-0
Emergency telephone No.:	Please contact the regional Merck representation in your country.

---

2. Composition/information on ingredients

CAS-No.:	174501-65-6
M:	226.02 g/mol
Formula Hill:	$C_8H_{15}BF_4N_2$

---

3. Hazards identification

Irritating to eyes and skin.

Caution! Substance not yet fully tested.

The test results available so far do not permit a complete evaluation. Further risks cannot be excluded if the product is handled inappropriately.

---

4. First aid measures

After inhalation: fresh air. Consult doctor if feeling unwell.
After skin contact: wash off with plenty of water. Remove contaminated clothing.
After eye contact: rinse out with plenty of water with the eyelid held wide open. Call in ophtalmologist.
After swallowing: immediately make victim drink plenty of water. Call in physician.

5. Fire-fighting measures

Suitable extinguishing media:
Water, CO_2, foam, powder.

Special risks:
Combustible. Development of hazardous combustion gases or vapours possible in the event of fire. The following may develop in event of fire: hydrogen fluoride, nitrogen oxides.

Special protective equipment for fire fighting:
Do not stay in dangerous zone without self-contained breathing apparatus. In order to avoid contact with skin, keep a safety distance and wear suitable protective clothing.

Other information:
Prevent fire-fighting water from entering surface water or groundwater. Contain escaping vapours with water.

6. Accidental release measures

Person-related precautionary measures:
Avoid substance contact. Do not inhale vapours/aerosols. Ensure supply of fresh air in enclosed rooms.

Environmental-protection measures:
Do not allow to enter sewerage system.

Procedures for cleaning / absorption:
Take up with liquid-absorbent material (e.g. Chemizorb®). Forward for disposal. Clean up affected area.

7. Handling and storage

Handling:

No further requirements.

Storage:

Tightly closed. At +15°C to +25°C.

8. Exposure controls/personal protection

Personal protective equipment:

Protective clothing should be selected specifically for the working place, depending on concentration and quantity of the hazardous substances handled. The resistance of the protective clothing to chemicals should be ascertained with the respective supplier.

Respiratory protection:	required when vapours/aerosols are generated.
Eye protection:	required

Hand protection:

In full contact:

Glove material:	nitrile rubber
Layer thickness:	0.40 mm
Breakthrough time:	> 480 Min.

In splash contact:

Glove material:	nitrile rubber
Layer thickness:	0.40 mm
Breakthrough time:	> 480 Min.

The protective gloves to be used must comply with the specifications of EC directive 89/686/EEC and the resultant standard EN374, for example KCL 730 Camatril® -Velours (full contact), 730 Camatril® -Velours (splash contact). The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.
This recommendation applies only to the product stated in the safety data sheet and supplied by us as well as to the purpose specified by us. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Industrial hygiene:
Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance.

9. Physical and chemical properties

viscosity ?

Form:		viscous		
Colour:		yellow to brown		
Odour:				
pH value		(20 °C)	5	
Melting point			-71 °C	
Boiling point			not available	
Ignition temperature			not available	
Flash point			not available	
Explosion limits	lower		not available	
	upper		not available	
Density			1.20 g/cm³	— after.
Solubility in Water			not available	

10. Stability and reactivity

Conditions to be avoided

Strong heating.

Substances to be avoided

strong oxidizing agents.

Hazardous decomposition products

in the event of fire: See chapter 5.

11. Toxicological information

Acute toxicity

Quantitative data on the toxicity of this product are not available.

Further toxicological information

After inhalation: Irritations of the mucous membranes, coughing, and dyspnoea.
After skin contact: Irritations.
After eye contact: Irritations.
After swallowing: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Other notes: The following applies to boron compounds in general: resorption is followed by nausea and vomiting, agitation, spasms, CNS disorders, cardiovascular disorders.

Further data

Further hazardous properties cannot be excluded.
The product should be handled with the care usual when dealing with chemicals.

12. Ecological information

Ecotoxic effects:
Quantitative data on the ecological effect of this product are not available.

Further ecologic data:
The following applies to boron compounds in general: biological effects: boric acid developing as a result of hydrolysis toxic for aquatic organisms; fish: Gambusia affinis 96 h. LC_{50}: 5600 mg/l; 24 h. LC_{50}:1800 mg/l; plants: as toxic from 1 mg/l .

Do not allow to enter waters, waste water, or soil!

13. Disposal considerations

Product:

Chemicals must be disposed of in compliance with the respective national regulations. Under www.retrologistik.de you will find country- and substance-specific information as well as contact partners.

Packaging:

Merck product packaging must be disposed of in compliance with the country-specific regulations or must be passed to a packaging return system. Under www.retrologistik.de you will find special information on the respective national conditions as well as contact partners.

14. Transport information

Not subject to transport regulations.

15. Regulatory information

Labelling according to EC Directives

Symbol:	Xi	Irritant
R-phrases:	36/38	Irritating to eyes and skin.
S-phrases:	---	
Additional labelling	Caution! Substance not yet fully tested.	

16. Other information

Reason for alteration

Chapter 9: change/addition in physical/chemical proprties.
Chapter 11: toxicological information.
Chapter 12: ecological information.

General update.

Regional representation:

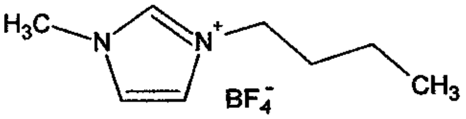
This information is given on the authorised Safety Data Sheet for your country.

MATERIAL SAFETY DATA SHEET

Product name	**1-Butyl-3-methylimidazolium tetrafluoroborate**	
MSDS code	BMITFB	
Revision date	29/04/2007	**Revision:** 3
Supersedes	06/10/2004	

1. Identification of the substance & the company

Chemical name 1-Butyl-3-methylimidazolium tetrafluoroborate



Synonym(s) bmim [BF_4], 1-Butyl-3-methyl-1H-imidazolium tetrafluoroborate

Chemical formula $C_8H_{15}N_2.\ BF_4$

CAS number 174501-65-6

Manufacturer

Chemada Fine Chemicals Ltd.
Nir Itzhak, D.N. HaNegev 85455, Israel.
Tel: +972-8-9983421/2

Supplier

- For Europe

ICL-IP Europe bv.
Fosfaatweg 48, 1013 BM Amsterdam, Netherlands
Tel: +31 20 8005800

- For USA

ICL-IP America, Inc.
95 MacCorkle Avenue SW, South Charleston, WV 25303-1411, USA.
Tel: 304-720-3950

- For Japan

ICL-IP Japan Ltd.
Izumi Shinkawa Building, 7th floor, 5-18, 1-chome Shinkawa, Chuo-ku,
Tokyo 104-0033, Japan
Tel: 03-3552-1611

Emergency telephone number:

- For Europe (+ 31) 115 689000

- For USA Chemtrec (800) 424-9300

- For Asia - Pacific

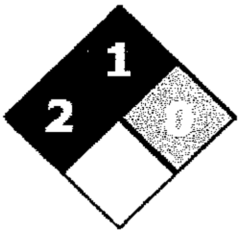
ALERT-SGS
24 hr Toll Free Number : +800 ALERTSGS (+800-2537-8747)
24 hr Singapore Exchange Number : +65 6542-9595

2. Hazards identification

mportant hazards Harmful if swallowed.
Irritant to eyes

NFPA Ratings (Scale 0-4)

- Health	2
- Fire	1
- Instability	0



3. Composition / information on ingredients

(Not Specifications)

Components	**Weight %**	**-EEC No.**	**EU Classification**	**Annex No.**
1-Butyl-3-methylimidazolium tetrafluoroborate 174501-65-6	98% min	Not Listed	Xn: R22 Xi: R36	None

This material is intended primarily for use as a solvent in the Pharmaceutical and other Fine Chemical Industries. Its use however is not limited to those stated.

4. First-aid measures

Eye contact Holding the eyelids apart, flush eyes promptly with copious flowing water for at least 20 minutes. Get medical attention immediately.

Skin contact Wash thoroughly with copious flowing water for at least 15 minutes. Wash clothing before reuse. Get medical attention immediately.

nhalation Keep him quiet and warm. Apply artificial respiration if necessary and get medical attention immediately.

ngestion DO NOT INDUCE VOMITING
If swallowed, wash mouth thoroughly with plenty of water and give water to drink.
Get medical attention immediately.

****

NOTE: Never give an unconscious person anything to drink.

****

After handling, wash before eating, drinking or smoking.

5. Fire - fighting measures

Flash point Not available

Flammable/Explosion limits

· **Lower (% vol)**	Not Determined
· **Upper (% vol)**	Not Determined
Auto-ignition temperature	Not available
Suitable extinguishing media	Carbon dioxide, dry chemicals, foam, water spray (fog).
Fire fighting procedure	Stay upwind. Avoid any bodily contact. Wear self-contained breathing apparatus in positive pressure mode and appropriate protective clothing. Wear full chemical protective suit if contact with material or dense fumes smoke anticipated.
Unusual fire and explosion hazards	None known

6. Accidental release measures

Personal precautions	Use approved respirator, chemical safety goggles, PVC gloves, boots and protective clothes.
Methods for cleaning up	Absorb on sand or vermiculite and place in closed container for disposal. Ventilate area and wash spill site after material pickup is complete.

7. Handling and storage

Handling	Handle in accordance with good industrial hygiene and safety procedures.
Storage	Store in a dry, cool, well-ventilated area

8. Exposure controls / personal protection

Exposure Limits :

Components	Weight %	ACGIH-TLV Data
1-Butyl-3-methylimidazolium tetrafluoroborate 174501-65-6	98% min	Not determined

Ventilation requirements	Mechanical ventilation is recommended. Use local exhaust at source of vapour.
Personal protective equipment:	
· **Respiratory protection**	Respirator with cartridge providing protection against acid gas-organic vapour or self-contained breathing apparatus. For short term exposure to low concentrations, an approved combination acid gas-organic vapour gas mask is suitable.
· **Hand protection**	PVC gloves
· **Eye protection**	Chemical safety goggles or face shield with safety glasses.
· **Skin and body protection**	Protective PVC clothing and boots

Hygiene measures	Do not eat, smoke or drink where material is handled, processed or stored. Wash hands carefully before eating or smoking.

9. Physical and chemical properties

Physical state	Liquid
Molecular weight	226.02
Density	1.22
Melting point/range	-71°C
Boiling point/range	Not available
Vapour pressure	Not available
Flash point	Not available
Solubility:	
Solubility in water	Miscible
Solubility in other solvents	Insoluble in most common organic solvents
Appearance	Clear, colourless viscous liquid

10. Stability and reactivity

Stability	Stable at normal conditions
Materials to avoid	No data available
Conditions to avoid	No data available
Hazardous decomposition products	No data available
Hazardous polymerization	Will not occur

11. Toxicological information

Acute toxicity:	
- Rat oral LD50	300 - 500 mg/Kg
- Rat dermal LD50	> 2000 mg/Kg
- Dermal irritation (rabbit)	Not irritant
- Dermal sensitization (LLNA)	Not a sensitizer
- Eye irritation (rabbit)	Mild irritant
Effects of overexposure:	Irritant to eyes
Chronic toxicity	No data available
Mutagenicity	Not mutagenic by the Ames Test

Carcinogenicity	Not classified as a carcinogen by USA OSHA Not classified by NTP Not classified by IARC

12. Ecological information

Aquatic toxicity	No information available
Mobility	This material is expected to have a low vapour pressure and air is not expected to be a major factor in its dispersal.
Persistence and degradability	This material is relatively stable under normal conditions

13. Disposal considerations

Waste from residues / unused products	Observe all federal, state and local environmental regulations when disposing of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

14. Transportation information

UN No.	Not regulated
MO	Not regulated
CAO/IATA	Not regulated
ADR/RID	Not regulated
UK	Not regulated
DOT	Not regulated

15. Regulatory information

Components	Weight %	-EEC No.	Annex No.
1-Butyl-3-methylimidazolium tetrafluoroborate 174501-65-6	98% min	Not Listed	None

Indication of danger	Harmful, symbol required (Xn)

R Phrases	R 22 :Harmful if swallowed. R 36 :Irritating to eyes.
S Phrases	S26- *In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.* S 39 :Wear eye/face protection.
SA	Not reported in the EPA TSCA Inventory
russels Tarrif No. (EU)	2933-29-90

6. Other information

ources of key data used	Toxic Substances Control Act (TSCA) Inventory, Pub: EPA, U.S.Government Printing Office, Washington, U.S.A. (Through STN Data Base). The European Inventory of Existing Chemical Substances, Pub: EEC, Office des Publications Officielles des Communautes Europeennes, Boite Postale 1003, L-1351, Luxembourg. (Through STN Data Base) Handbook of Existing & New Chemical Substances, Editor: Chemical Products Safety Division, Basic Industries Bureau, Ministry of International Trade & Industries, Tokyo, Japan. (Through STN Data Base)
his data sheet contains changes rom the previous version in ection(s)	14
SDS valid until	30/04/2010

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lthough the information and recommendations set forth herein (herinafter "information") are presented in good faith and elieved to be correct as of the date hereof, Chemada makes no representations as to the completeness or accuracy hereof.
nformation is supplied upon the condition that the persons receiving same will make their own determination as to its afety and suitability for their purposes prior to use.
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mail: msds@chemada.com
ttp://www.chemada.com

End of safety data sheet

BOC GASES

MATERIAL SAFETY DATA SHEET

PRODUCT NAME: CARBON DIOXIDE, GAS

1. Chemical Product and Company Identification

BOC Gases,
Division of
The BOC Group, Inc.
575 Mountain Avenue
Murray Hill, NJ 07974

TELEPHONE NUMBER: (908) 464-8100
24-HOUR EMERGENCY TELEPHONE NUMBER:
CHEMTREC (800) 424-9300

BOC Gases
Division of
BOC Canada Limited
5975 Falbourne Street, Unit 2
Mississauga, Ontario L5R 3W6

TELEPHONE NUMBER: (905) 501-1700
24-HOUR EMERGENCY TELEPHONE NUMBER:
(905) 501-0802
EMERGENCY RESPONSE PLAN NO: 20101

PRODUCT NAME: CARBON DIOXIDE, GAS
CHEMICAL NAME: Carbon Dioxide
COMMON NAMES/SYNONYMS: Carbonic Anhydride
TDG (Canada) CLASSIFICATION: 2.2
WHMIS CLASSIFICATION: A

PREPARED BY: Loss Control (908)464-8100/(905)501-1700
PREPARATION DATE: 6/1/95
REVIEW DATES: 6/7/96

2. Composition, Information on Ingredients

INGREDIENT	% VOLUME	PEL-OSHA[1]	TLV-ACGIH[2]	LD_{50} or LC_{50} Route/Species
Carbon Dioxide FORMULA: CO_2 CAS: 124-38-9 RTECS #: FF6400000	99.8 TO 99.999	5000 ppm TWA	5000 ppm TWA 30,000 ppm STEL	Not Available

[1] As stated in 29 CFR 1910, Subpart Z (revised July 1, 1993)

[2] As stated in the ACGIH 1994-95 Threshold Limit Values for Chemical Substances and Physical Agents

3. Hazards Identification

EMERGENCY OVERVIEW

Oxygen levels below 19.5% may cause asphyxia. Carbon dioxide exposure can cause nausea and respiratory problems. High concentrations may cause vasodilation leading to circulatory collapse.

ROUTE OF ENTRY:

Skin Contact	Skin Absorption	Eye Contact	Inhalation	Ingestion
Yes	No	Yes	Yes	Yes

HEALTH EFFECTS:

Exposure Limits Yes	Irritant No	Sensitization No
Teratogen No	Reproductive Hazard No	Mutagen No
Synergistic Effects None reported		

Carcinogenicity: – NTP: No IARC: No OSHA: No

EYE EFFECTS:
No adverse effects anticipated.

SKIN EFFECTS:
No adverse effects anticipated.

INGESTION EFFECTS:
No adverse effects anticipated.

INHALATION EFFECTS:
Carbon dioxide is the most powerful cerebral vasodilator known. Inhaling large concentrations causes rapid circulatory insufficiency leading to coma and death. Asphyxiation is likely to occur before the effects of carbon dioxide overexposure. Chronic, harmful effects are not known from repeated inhalation of low concentrations. Low concentrations of carbon dioxide cause increased respiration and headache.

Effects of oxygen deficiency resulting from simple asphyxiants may include: rapid breathing, diminished mental alertness, impaired muscular coordination, faulty judgement, depression of all sensations, emotional instability, and fatigue. As asphyxiation progresses, nausea, vomiting, prostration, and loss of consciousness may result, eventually leading to convulsions, coma, and death.

Oxygen deficiency during pregnancy has produced developmental abnormalities in humans and experimental animals.

NFPA HAZARD CODES		**HMIS HAZARD CODES**		**RATINGS SYSTEM**
Health:	1	Health:	1	0 = No Hazard
Flammability:	0	Flammability:	0	1 = Slight Hazard
Reactivity:	0	Reactivity:	0	2 = Moderate Hazard
				3 = Serious Hazard
				4 = Severe Hazard

4. First Aid Measures

EYES:
Never introduce oil or ointment into the eyes without medical advice! If pain is present, refer the victim to an ophthalmologist for further treatment and follow up.

SKIN:
No adverse effects anticipated.

INGESTION:
Not anticipated.

INHALATION:
PROMPT MEDICAL ATTENTION IS MANDATORY IN ALL CASES OF OVEREXPOSURE TO CARBON DIOXIDE. RESCUE PERSONNEL SHOULD BE EQUIPPED WITH SELF-CONTAINED BREATHING APPARATUS. Conscious persons should be assisted to an uncontaminated area and inhale fresh air. Quick removal from the contaminated area is most important. Unconscious persons should be moved to an uncontaminated area, given mouth-to-mouth resuscitation and supplemental oxygen. Further treatment should be symptomatic and supportive.

5. Fire Fighting Measures

Conditions of Flammability: Nonflammable		
Flash point: None	*Method:* Not Applicable	*Autoignition* Temperature: None
LEL(%): None	UEL(%): None	
Hazardous combustion products: None		
Sensitivity to mechanical shock: None		
Sensitivity to static discharge: None		

FIRE AND EXPLOSION HAZARDS:
None. Nonflammable

6. Accidental Release Measures

Evacuate all personnel from affected area. Use appropriate protective equipment. If leak is in user's equipment, be certain to purge piping with inert gas prior to attempting repairs. If leak is in container or container valve, contact the appropriate emergency telephone number listed in Section 1 or call your closest BOC location.

7. Handling and Storage

Electrical Classification:
Non-Hazardous

Dry carbon dioxide can be handled in most common structural materials. Moist carbon dioxide is generally corrosive by its formation of carbonic acid. For applications with moist Carbon Dioxide, 316, 309 and 310 stainless steels may be used as well as Hastelloy ® A, B, & C, and Monel ®. Ferrous Nickel alloys are slightly susceptible to corrosion. At normal temperatures carbon dioxide is compatible with most plastics and elastomers.

Use only in well-ventilated areas. Carbon dioxide vapor is heavier than air and will accumulate in low areas. Valve protection caps must remain in place unless container is secured with valve outlet piped to use point. Do not drag, slide or roll cylinders. Use a suitable hand truck for cylinder movement. Use a pressure reducing regulator when connecting cylinder to lower pressure (<3000 psig) piping or systems. Do not heat cylinder by any means to increase the discharge rate of product from the cylinder. Use a check valve or trap in the discharge line to prevent hazardous back flow into the system.

Protect cylinders from physical damage. Store in cool, dry, well-ventilated area away from heavily trafficked areas and emergency exits. Do not allow the temperature where cylinders are stored to exceed 125°F (52°C). Cylinders should be stored upright and firmly secured to prevent falling or being knocked over. Full and empty cylinders should be segregated. Use a "first in-first out" inventory system to prevent full cylinders being stored for excessive periods of time.

For additional storage recommendations, consult Compressed Gas Association's Pamphlet P-1.

Never carry a compressed gas cylinder or a container of a gas in cryogenic liquid form in an enclosed space such as a car trunk, van or station wagon. A leak can result in a fire, explosion, asphyxiation or a toxic exposure.

Maximum use for potable water 100 mg/l.

8. Exposure Controls, Personal Protection

EXPOSURE LIMITS[1]:

INGREDIENT	% VOLUME	PEL-OSHA[2]	TLV-ACGIH[3]	LD_{50} or LC_{50} Route/Species
Carbon Dioxide FORMULA: CO_2 CAS: 124-38-9 RTECS #: FF6400000	99.8 TO 99.999	5000 ppm TWA	5000 ppm TWA 30,000 ppm STEL	Not Available

[1] Refer to individual state of provincial regulations, as applicable, for limits which may be more stringent than those listed here.
[2] As stated in 29 CFR 1910, Subpart Z (revised July 1, 1993)
[3] As stated in the ACGIH 1994-1995 Threshold Limit Values for Chemical Substances and Physical Agents.

IDLH (Carbon Dioxide): 50,000 ppm

ENGINEERING CONTROLS:
Use local exhaust to prevent accumulation of high concentrations so as to reduce the oxygen level in the air to less than 19.5% and the carbon dioxide concentration below the exposure limit.

EYE/FACE PROTECTION:
Safety goggles or glasses as appropriate for the job.

SKIN PROTECTION:
Protective gloves of any material appropriate for the job.

RESPIRATORY PROTECTION:

Positive pressure air line with full-face mask and escape bottle or self-contained breathing apparatus should be available for emergency use.

OTHER/GENERAL PROTECTION:
Safety shoes.

9. Physical and Chemical Properties

PARAMETER	VALUE	UNITS
Physical state (gas, liquid, solid)	: Gas	
Vapor pressure at 70 °F	: 856	psia
Vapor density at 70 °F, 1 atm (Air = 1)	: 1.53	
Evaporation point	: Not Available	
Boiling point (CO2 Sublimes)	: -109.3	°F
	: -78.5	°C
Freezing point	: -69.8	°F
	: -56.6	°C
pH	: Not Available	
Specific gravity	*: Not Available*	
Oil/water partition coefficient	: Not Available	
Solubility (H20)	: Very soluble	
Odor threshold	: Not Applicable	
Odor and appearance	: A colorless, odorless gas.	

10. Stability and Reactivity

STABILITY:
Stable

INCOMPATIBLE MATERIALS:
Certain reactive metals, hydrides, moist cesium monoxide, or lithium acetylene carbide diammino may ignite. Passing carbon dioxide over a mixture of sodium peroxide and aluminum or magnesium may explode.

HAZARDOUS DECOMPOSITION PRODUCTS:
Carbon monoxide and oxygen when heated above 3092 °F (1700°C). Carbonic acid is formed in the presence of moisture.

HAZARDOUS POLYMERIZATION:
Will not occur.

11. Toxicological Information

REPRODUCTIVE:
Oxygen deficiency during pregnancy has produced developmental abnormalities in humans and experimental animals.

Exposure of female rats to 60,000 ppm carbon dioxide for 24 hours has produced toxic effects to the embryo and fetus in pregnant rats. Toxic effects to the reproductive system have been observed in other mammalian species at similar concentrations.

OTHER:

Carbon dioxide is the most powerful cerebral vasodilator known. Inhaling large concentrations causes rapid circulatory insufficiency leading to coma and death. Chronic, harmful effects are not known from repeated inhalation of low (3 to 5 molar %) concentrations.

12. Ecological Information

No data given.

13. Disposal Considerations

Do not attempt to dispose of residual waste or unused quantities. Return in the shipping container PROPERLY LABELED, WITH ANY VALVE OUTLET PLUGS OR CAPS SECURED AND VALVE PROTECTION CAP IN PLACE to BOC Gases or authorized distributor for proper disposal.

14. Transport Information

PARAMETER	United States DOT	Canada TDG
PROPER SHIPPING NAME:	Carbon Dioxide	Carbon Dioxide
HAZARD CLASS:	2.2	2.2
IDENTIFICATION NUMBER:	UN 1013	UN 1013
SHIPPING LABEL:	NONFLAMMABLE GAS	NONFLAMMABLE GAS

15. Regulatory Information

SARA TITLE III NOTIFICATIONS AND INFORMATION

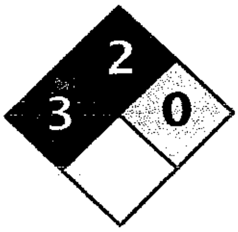
SARA TITLE III HAZARD CLASSES:
Acute Health Hazard
Sudden Release of Pressure Hazard

16. Other Information

Compressed gas cylinders shall not be refilled without the express written permission of the owner. Shipment of a compressed gas cylinder which has not been filled by the owner or with his/her (written) consent is a violation of transportation regulations.

DISCLAIMER OF EXPRESSED AND IMPLIED WARRANTIES:
Although reasonable care has been taken in the preparation of this document, we extend no warranties and make no representations as to the accuracy or completeness of the information contained herein, and assume no responsibility regarding the suitability of this information for the user's intended purposes or for the consequences of its use. Each individual should make a determination as to the suitability of the information for their particular purpose(s).

ScienceLab.com
Chemicals & Laboratory Equipment



Health	3
Fire	2
Reactivity	0
Personal Protection	H

Material Safety Data Sheet
Monoethanolamine MSDS

Section 1: Chemical Product and Company Identification

duct Name: Monoethanolamine

talog Codes: SLA4792, SLA2452, SLA3955

S#: 141-43-5

ECS: KJ5775000

CA: TSCA 8(b) inventory: Ethanolamine

: Not applicable.

nonym: Colamine, Glycinol, Olamine; Ethanolamine; minoethanol; 2-Hydroxyethylamine; beta-Ethanolamine; a-Hydroxyethylamine

emical Name: Ethanol 2-amino

emical Formula: HOCH2CH2NH2 or C2-H7-N-O

Contact Information:

Sciencelab.com, Inc.
14025 Smith Rd.
Houston, Texas 77396

US Sales: **1-800-901-7247**
International Sales: **1-281-441-4400**

Order Online: ScienceLab.com

CHEMTREC (24HR Emergency Telephone), call:
1-800-424-9300

International CHEMTREC, call: 1-703-527-3887

For non-emergency assistance, call: 1-281-441-4400

Section 2: Composition and Information on Ingredients

mposition:

ame	CAS #	% by Weight
thanolamine	141-43-5	100

xicological Data on Ingredients: Ethanolamine: ORAL (LD50): Acute: 1720 mg/kg [Rat.]. 700 mg/kg [Mouse]. DERMAL 50): Acute: 1000 mg/kg [Rabbit.].

Section 3: Hazards Identification

tential Acute Health Effects:
ry hazardous in case of eye contact (irritant), of ingestion, . Hazardous in case of skin contact (irritant, rmeator), of inhalation (lung irritant). Slightly hazardous in case of skin contact (corrosive), of eye contact rrosive). Liquid or spray mist may produce tissue damage particularly on mucous membranes of eyes, mouth d respiratory tract. Skin contact may produce burns. Inhalation of the spray mist may produce severe irritation respiratory tract, characterized by coughing, choking, or shortness of breath. Inflammation of the eye is aracterized by redness, watering, and itching.

tential Chronic Health Effects:
RCINOGENIC EFFECTS: Not available.
UTAGENIC EFFECTS: Not available.
RATOGENIC EFFECTS: Not available.

VELOPMENTAL TOXICITY: Not available.
ı substance may be toxic to kidneys, lungs, liver, central nervous system (CNS).
ɔeated or prolonged exposure to the substance can produce target organs damage. Repeated or prolonged
ıtact with spray mist may produce chronic eye irritation and severe skin irritation. Repeated or prolonged
ɪosure to spray mist may produce respiratory tract irritation leading to frequent attacks of bronchial infection.

Section 4: First Aid Measures

ı Contact:
ɘck for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes,
ɪping eyelids open. Cold water may be used. Get medical attention immediately. Finish by rinsing thoroughly
ı running water to avoid a possible infection.

n Contact:
ɔase of contact, immediately flush skin with plenty of water for at least 15 minutes while removing contaminated
thing and shoes. Cover the irritated skin with an emollient. Cold water may be used.Wash clothing before
se. Thoroughly clean shoes before reuse. Get medical attention immediately.

rious Skin Contact:
ısh with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek immediate
dical attention.

ıalation:
ıhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get
dical attention.

rious Inhalation:
ɔcuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or
istband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth
ıuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation
en the inhaled material is toxic, infectious or corrosive. Seek immediate medical attention.

ıestion:
NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an
ɔonscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight
thing such as a collar, tie, belt or waistband.

rious Ingestion: Not available.

Section 5: Fire and Explosion Data

ımmability of the Product: Combustible.

ıto-Ignition Temperature: 410°C (770°F)

ısh Points: CLOSED CUP: 86°C (186.8°F). OPEN CUP: 93.34°C (200°F) (Cleveland).

ımmable Limits: LOWER: 3% UPPER: 23.5%

ɔducts of Combustion: These products are carbon oxides (CO, CO2), nitrogen oxides (NO, NO2...).

'e Hazards in Presence of Various Substances:
ımmable in presence of open flames and sparks, of heat.
ɪn-flammable in presence of shocks.

ıplosion Hazards in Presence of Various Substances:
ɔks of explosion of the product in presence of mechanical impact: Not available.
ɔks of explosion of the product in presence of static discharge: Not available.

'e Fighting Media and Instructions:

ALL FIRE: Use DRY chemical powder.
ℜGE FIRE: Use water spray, fog or foam. Do not use water jet.

ecial Remarks on Fire Hazards: Not available.

ecial Remarks on Explosion Hazards: Not available.

Section 6: Accidental Release Measures

iall Spill:
ıte with water and mop up, or absorb with an inert dry material and place in an appropriate waste disposal itainer. If necessary: Neutralize the residue with a dilute solution of acetic acid.

ge Spill:
mbustible material. Corrosive liquid.
ep away from heat. Keep away from sources of ignition. Stop leak if without risk. Absorb with DRY earth, ıd or other non-combustible material. Do not get water inside container. Do not touch spilled material. Use ter spray curtain to divert vapor drift. Prevent entry into sewers, basements or confined areas; dike if needed. ll for assistance on disposal. Neutralize the residue with a dilute solution of acetic acid. Be careful that the duct is not present at a concentration level above TLV. Check TLV on the MSDS and with local authorities.

Section 7: Handling and Storage

ecautions:
ep container dry. Keep away from heat. Keep away from sources of ignition. Ground all equipment containing terial. Do not ingest. Do not breathe gas/fumes/ vapor/spray. Never add water to this product. In case of ufficient ventilation, wear suitable respiratory equipment. If ingested, seek medical advice immediately and ›w the container or the label. Avoid contact with skin and eyes. Keep away from incompatibles such as dizing agents, acids.

rage:
ep container in a cool, well-ventilated area. Keep container tightly closed and sealed until ready for use. Avoid possible sources of ignition (spark or flame). Sensitive to light. Store in light-resistant containers.
groscopic

Section 8: Exposure Controls/Personal Protection

gineering Controls:
›vide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapors below their pective threshold limit value. Ensure that eyewash stations and safety showers are proximal to the rk-station location.

rsonal Protection:
ce shield. Full suit. Vapor respirator. Be sure to use an approved/certified respirator or equivalent. Gloves. ots.

rsonal Protection in Case of a Large Spill:
lash goggles. Full suit. Vapor respirator. Boots. Gloves. A self contained breathing apparatus should be ed to avoid inhalation of the product. Suggested protective clothing might not be sufficient; consult a specialist FORE handling this product.

posure Limits:
/A: 3 STEL: 5 (ppm) [United Kingdom (UK)]
/A: 3 STEL: 6 (ppm) from ACGIH (TLV) [United States]
EL: 15 (mg/m3) from NIOSH [United States]
/A: 3 STEL: 6 (ppm) from NIOSH [United States]
/A: 3 (ppm) from OSHA (PEL) [United States]
/A: 6 (mg/m3) from OSHA (PEL) [United States]

NTSMAN

MATERIAL SAFETY DATA SHEET

READ AND UNDERSTAND MATERIAL SAFETY DATA SHEET BEFORE HANDLING OR DISPOSING OF PRODUCT

)UCT CODE AND NAME : MEA MONOETHANOLAMINE, MEA
E DATE : 03/27/2000
S CD DATE : 7/1/2000

IEMICAL PRODUCT AND COMPANY IDENTIFICATION

RIAL IDENTITY

'RODUCT CODE AND NAME

MEA MONOETHANOLAMINE, MEA

hemical Name and/or Family or Description:

Alkanolamine

OMPANY INFORMATION

Huntsman Petrochemical Corporation
P.O. Box 27707
Houston, TX 77227-7707

TELEPHONE NUMBERS
Transportation Emergency
Company: (409) 727-0831
CHEMTREC: (800) 424-9300
Medical Emergency: (409) 722-9673 (24 Hour)
General MSDS Assistance: (713) 235-6432
Technical Information: (512) 459-6543

)MPOSITION AND INFORMATION ON INGREDIENTS

RITERIA FOR LISTING COMPONENTS IN THE COMPOSITION SECTION ARE AS FOLLOWS: CARCINOGENS ARE LISTED WHEN NT AT 0.1 % OR GREATER; COMPONENTS WHICH ARE OTHERWISE HAZARDOUS ACCORDING TO OSHA ARE LISTED WHEN NT AT 1.0 % OR GREATER; NON-HAZARDOUS COMPONENTS ARE LISTED AT 3.0 % OR GREATER. THIS IS NOT INTENDED COMPLETE COMPOSITIONAL DISCLOSURE. REFER TO SECTION 14 FOR APPLICABLE STATES' RIGHT TO KNOW AND REGULATORY INFORMATION.

t and/or Component(s) Carcinogenic According to:

IARC NTP OTHER NONE X

ition:

al Name	CAS Number	Exposure Limits	Range in %
, 2-amino-	141-43-5	6 ppm STEL-ACGIH 3 ppm TWA-OSHA 6 ppm STEL-OSHA 3 ppm TWA-ACGIH	100

'RODUCT IS CONSIDERED HAZARDOUS ACCORDING TO OSHA (1910.1200).

ɩUCT CODE AND NAME : MEA MONOETHANOLAMINE, MEA
: DATE : 03/27/2000
CD DATE : 7/1/2000
ɂANY : HUNTSMAN

ZARD IDENTIFICATION

ɜENCY OVERVIEW

arance:

lear liquid

:

mmonia-like odor

WARNING STATEMENT

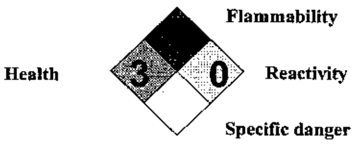
ANGER !

CORROSIVE - CAUSES EYE AND SKIN BURNS
HARMFUL OR FATAL IF SWALLOWED
MAY CAUSE DIZZINESS AND DROWSINESS
CAUSES RESPIRATORY TRACT IRRITATION AND CAN CAUSE DAMAGE
ASPIRATION HAZARD IF SWALLOWED -
CAN ENTER LUNGS AND CAUSE DAMAGE
MAY CAUSE LIVER AND KIDNEY DAMAGE BASED ON ANIMAL DATA

[azardous Material ıformation System Jnited States)

Health	3
Fire	1
Reactivity	0
Personal protection	

National Fire Protection Association NFPA (United States)



TIAL HEALTH EFFECTS

Route of Exposure

e X **Skin** X **Inhalation** X **Ingestion**

ɩf Overexposure

e:

Eyes: Causes irritation, experienced as pain, with excess blinking and tear production, and seen as extreme redness and swelling of the eye and chemical burns of the eye. Severe eye damage may cause blindness.

Skin: Causes severe irritation with pain, severe excess redness and swelling with chemical burns, blister formation, and possible tissue destruction. Other than the potential skin irritation effects noted above, acute (short term) adverse effects are not expected from brief skin contact; see other effects, below, and Section 11 for information regarding potential long term effects.

Inhalation: Vapors or mist, especially as generated from heating the material or as from exposure in poorly ventilated areas or confined spaces, are irritating and cause nasal discharge, coughing, and discomfort in nose and throat. Prolonged or repeated overexposure may result in lung damage. Inhalation may cause dizziness, drowsiness, euphoria, loss of coordination, disorientation, headache, nausea, and vomiting. In poorly ventilated areas or confined spaces, unconsciousness and asphyxiation may result. Prolonged or repeated overexposure may result in the absorption of potentially harmful amounts of material.

Ingestion: Causes burning of mouth, throat, and stomach with abdominal and chest pain, nausea, vomiting, diarrhea, thirst, weakness, and collapse. Aspiration may occur during swallowing or vomiting, resulting in lung damage.

Sensitization Properties: Unknown

ɩnic:

ɘpeated skin contact may cause a persistent irritation or dermatitis. Repeated inhalation may cause lung damage.

ical Conditions Aggravated by Exposure:

kin contact may aggravate an existing dermatitis (skin condition). Overexposure to vapor, dust or mist may aggravate isting respiratory conditions, such as asthma, bronchitis, and inflammatory or fibrotic respiratory disease. Repeated erexposure may aggravate existing liver or kidney disease.

r Remarks:

his product contains one or more amines which may produce temporary and reversible hazy or blurred vision. Symptoms sappear when exposure is terminated.

ST AID MEASURES

nmediately flush eyes with large amounts of running water for at least 15 minutes. Hold eyelids apart while flushing to rinse entire rface of eye and lids with water. Do not attempt to neutralize with chemical agents. Obtain medical attention immediately. Continue shing for an additional 15 minutes if medical attention is not immediately available.

nmediately remove contaminated clothing and shoes. Under a safety shower, flush skin thoroughly with large amounts of running ater for at least 15 minutes. Do not attempt to neutralize with chemical agents. Get medical attention immediately. Discard or contaminate clothing and shoes before reuse.

n:

person is conscious and can swallow, immediately give two glasses of water (16 oz.) but do not induce vomiting. This material is rrosive. If vomiting occurs, give fluids again. Have a physician determine if condition of patient will permit induction of vomiting or acuation of stomach. Do not give anything by mouth to an unconscious or convulsing person.

ion:

inhaled, remove to fresh air. If not breathing or in respiratory distress, clear person's airway and start artificial respiration. With a ysician's advice, give supplemental oxygen using a bag-valve mask or manually triggered oxygen supply.

nstructions:

wallowing of this corrosive material may result in severe ulceration, inflammation, and possible perforation of the upper imentary tract, with hemorrhage and fluid loss. Aspiration of this product during induced emesis can result in severe lung jury. If evacuation of stomach is necessary, use method least likely to cause aspiration, such as gastric lavage after dotracheal intubation. Contact a Poison Control Center for additional treatment information.

E-FIGHTING MEASURES

Temperature - AIT (degrees C):

ot determined.

oint (degrees C):

.5 (204 F) (PMCC)

ble Limits % (Lower-Upper):

wer: 5
per: 17

nended Fire Extinguishing Agents And Special Procedures:

se water spray, dry chemical, foam, or carbon dioxide to extinguish flames. Use water spray to cool fire-exposed containers. Water foam may cause frothing.

l or Explosive Hazards:

one

Protective Equipment for Firefighters:

ear special chemical protective clothing and positive pressure self-contained breathing apparatus. Approach fire from upwind to oid hazardous vapors and toxic decomposition products. Decontaminate or discard any clothing that may contain chemical residues.

'UCT CODE AND NAME : MEA MONOETHANOLAMINE, MEA
: DATE : 03/27/2000
: CD DATE : 7/1/2000
'ANY : HUNTSMAN

'CIDENTAL RELEASE MEASURES (Transportation Spills: CHEMTREC (800)424-9300)

:res in Case of Accidental Release, Breakage or Leakage:

entilate area. Avoid breathing vapor. Wear appropriate personal protective equipment, including appropriate respiratory protection. ›ntain spill if possible. Wipe up or absorb on suitable material and shovel up. Prevent entry into sewers and waterways. Avoid ntact with skin, eyes or clothing.

NDLING AND STORAGE

ions to be Taken in

ing:

inimum feasible handling temperatures should be maintained. Eye wash and safety shower should be available nearby when this ɔduct is handled or used.

e:

ɘriods of exposure to high temperatures should be minimized. Water contamination should be avoided.

POSURE CONTROLS/PERSONAL PROTECTION

ve Equipment (Type)

ıce Protection:

ᵥoid eye contact. Chemical type goggles with face shield must be worn. Do not wear contact lenses.

rotection:

rotective clothing such as coveralls or lab coats must be worn. Launder or dry-clean when soiled. Gloves resistant to chemicals and troleum distillates required. When handling large quantities, impervious suits, gloves, and rubber boots must be worn.

emove and dry-clean or launder clothing soaked or soiled with this material before reuse. Dry cleaning of contaminated clothing may more effective than normal laundering. Inform individuals responsible for cleaning of potential hazards associated with handling ntaminated clothing.

atory Protection:

irborne concentrations should be kept to lowest levels possible. If vapor, mist or dust is generated and the occupational posure limit of the product, or any component of the product, is exceeded, use appropriate NIOSH or MSHA approved air rifying or air supplied respirator after determining the airborne concentration of the contaminant. Air supplied respirators ould always be worn when airborne concentration of the contaminant or oxygen content is unknown.

ıtion:

ɿequate to meet occupational exposure limits (see below).

ıre Limit for the Total Product:

onoethanolamine (ethanolamine): OSHA PEL-TWA 3.0 ppm; STEL 6.0 ppm ACGIH TLV-TWA 3.0 ppm; STEL) ppm

YSICAL AND CHEMICAL PROPERTIES

ınce:

ıear liquid

ımmonia-like odor

Point (degrees C):

0.5 (339 F)

/Freezing Point (degrees C):

.5 (51 F)

: Gravity (water=1):

)2

3

ressure:

nmHg at 20 C (68 F)

/:

3 cSt at 20 C (68 F)

ntent:

6 by ASTM D 2369

ensity (Air=1):

y in Water (%):

)

ne

TABILITY AND REACTIVITY

ıterial Reacts Violently With:

r **Water** **Heat** **Strong Oxidizers** **Others** X **None of these**

nts:

his material reacts violently with acids.

s Evolved When Subjected to Heat or Combustion:

oxic levels of ammonia, combustion products of nitrogen, carbon monoxide, carbon dioxide, irritating aldehydes and ketones may be med on burning in a limited air supply.

ous Polymerizations:

O NOT OCCUR

OXICOLOGICAL INFORMATION

OLOGICAL INFORMATION (ANIMAL TOXICITY DATA)

al:
)50 Believed to be > 1.00 - 2.00 g/kg (rat) moderately toxic
ıalation:
ot determined.
ırmal:
)50 > 1.00 g/kg (rabbit) slightly toxic

.TION INDEX, ESTIMATION OF IRRITATION (SPECIES)

kin:
Draize) Believed to be > 6.50 - 8.00 /8.0 (rabbit) corrosive
yes:
Draize) Believed to be > 80.00 - 110.00 /110 (rabbit) extremely irritating
ensitization:
lot determined.

'rolonged and repeated ingestion of monoethanolamine has caused kidney and liver damage in laboratory animals. In ddition, a developmental toxicity study, using unconventional statistical treatment of the data, demonstrated developmental xicity in rats. The true signifigance of the study data is not clear, since a full re-interpretation of this data is not possible at is time. Additional or repeat studies are planned or underway to better define the toxic potential of this product, or to verify e results obtained from previous animal studies.

'ISPOSAL CONSIDERATIONS:

)isposal Methods:

'his product has been evaluated for RCRA characteristics and does not meet the criteria of a hazardous waste if discarded in its ırchased form. Under RCRA, it is the responsibility of the user of the product to determine at the time of disposal, whether the oduct meets RCRA criteria for hazardous waste. This is because product uses, transformations, mixtures, processes, etc. may nder the resulting materials hazardous.

ιs:

lone

RANSPORT INFORMATION

ortation

r Shipping Name:
thanolamine

d Class:

fication Number:
N 2491

ng Group:

Required:
orrosive

;

per Shipping Name:
ot evaluated

per Shipping Name:
ot evaluated

per Shipping Name:
thanolamine

ard Class:

tification Number:

\ 2491

›el Required:
orrosive

EGULATORY INFORMATION

Regulations:

Title III:

on 302/304 Extremely Hazardous Substances

nical Name	CAS Number	Range in %	TPQ	RQ
e.				

on 311 Hazardous Categorization:

:e X Chronic X Fire Pressure Reactive N/A

on 313 Toxic Chemical

nical Name	CAS Number	Concentration
ə.		

LA 102(a)/DOT Hazardous Substances:

nical Name	CAS Number	Range in %	RQ
ə.			

Right-to-Know Regulations:

mical Name	State Right-to-know
ɜnol, 2-amino-	CT, FL, IL, MA, NJ, PA, RI

State list: CT (Connecticut), FL (Florida), IL (Illinois), MI (Michigan), LA (Louisiana), MA (Massachusetts), NJ (New Jersey), PA (Pennsylvania), RI (Rhode Island)

‑nia Prop. 65:
›llowing detectable components of this product are substances, or belong to classes of substances, known to the State of ‑nia to cause cancer and/or reproductive toxicity.

ıical Name	CAS Number
e.	

ιNATIONAL REGULATIONS:

Inventory Status:

; product, or its components, are listed on or are exempt from the the Toxic Substance Control Act (TSCA) Chemical stance Inventory.

S Classification:

ɜs E: Corrosive

an Inventory Status:

product, or its components, are listed on or are exempt from the Canadian Domestic Substance List (DSL).

:S Inventory Status:

product, or its components, are listed on or are exempt from the European Inventory of Existing Chemical Substances (EINECS) or :uropean List of Notified Chemical Substances (ELINCS).

lian Inventory Status:

product, or its components, are listed on or are exempt from the Australian Inventory of Chemical Substances (AICS).

UCT CODE AND NAME : MEA MONOETHANOLAMINE, MEA
DATE : 03/27/2000
CD DATE : 7/1/2000
ANY : HUNTSMAN

Inventory Status:

s product, or its components, are listed on or are exempt from the Japan Ministry of International Trade and Industry (MITI) ntory.

NVIRONMENTAL INFORMATION

Toxicity:

C50-96hr Aquatic toxicity rating is > 100.00 - 1000.00 ppm practically non-toxic

:

is product is expected to be mobile in soil and not be expected to adsorb to suspended solids or sediments in water.

nce and Biodegradability:

his product undergoes moderate biodegradation and is not expected to be persistent in the environment.

l to Bioaccumulate:

his product is not expected to bioaccumulate. K_{OW} = -1.31

s:

one

THER INFORMATION 03/27/2000

des: 7/30/97 **The following section has been revised: 11**

te: 06/09/2000

FORMATION IN THIS DATA SHEET IS PROVIDED INDEPENDENTLY OF ANY SALE OF THE PRODUCT. IT IS PROVIDED
IE PURPOSE OF HAZARD COMMUNICATION AS PART OF HUNTSMAN'S PRODUCT SAFETY PROGRAM. IT IS INTENDED
IS A GUIDE TO THE APPROPRIATE PRECAUTIONARY HANDLING OF THE PRODUCT BY A PROPERLY TRAINED PERSON.
E ENCOURAGED AND REQUESTED TO ADVISE THOSE WHO MAY COME IN CONTACT WITH SUCH PRODUCTS OF THE
MATION CONTAINED HEREIN. THE DATA RELATES ONLY TO THE SPECIFIC PRODUCT DESIGNATED, AND DOES NOT
E TO USE OF THE PRODUCT IN COMBINATION WITH ANY OTHER MATERIAL OR USE OF THE PRODUCT IN ANY
SS. THE DATA IS NOT INTENDED TO CONSTITUTE PERFORMANCE INFORMATION CONCERNING THE PRODUCT. NO
SS WARRANTY, OR IMPLIED WARRANTY OF MERCHANTABILITY FOR FITNESS FOR A PARTICULAR PURPOSE IS MADE
ESPECT TO THE PRODUCT, ITS COMPOSITION, ITS SAFETY OR THE INFORMATION CONTAINED IN THIS DATA SHEET.

ERMINE THE APPLICABILITY OR THE EFFECTS OF ANY LAW OR REGULATION WITH RESPECT TO THE PRODUCT,
ER SHOULD CONSULT A LEGAL ADVISOR OR THE APPROPRIATE GOVERNMENT AGENCY. HUNTSMAN DOES NOT
TAKE TO FURNISH ADVICE ON SUCH MATTERS.

NT DATA SHEETS ARE AVAILABLE FOR ALL HUNTSMAN PRODUCTS. YOU ARE URGED TO OBTAIN DATA SHEETS FOR
NTSMAN PRODUCTS YOU BUY, USE OR DISTRIBUTE BY CALLING (713) 235-6432 OR DIRECTING YOUR INQUIRIES TO:

HUNTSMAN
COORDINATOR, PRODUCT SAFETY
O. Box 27707
HOUSTON, TX 77227-7707

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APPENDIX

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2.8.16 C —
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Infrared Spectroscopy

IR Absorptions for Representative Functional Groups

Functional Group	Molecular Motion	Wavenumber (cm^{-1})
alkanes	C-H stretch	2950-2800
	CH_2 bend	~1465
	CH_3 bend	~1375
	CH_2 bend (4 or more)	~720
alkenes	=CH stretch	3100-3010
	C=C stretch (isolated)	1690-1630
	C=C stretch (conjugated)	1640-1610
	C-H in-plane bend	1430-1290
	C-H bend (monosubstituted)	~990 & ~910
	C-H bend (disubstituted - E)	~970
	C-H bend (disubstituted - 1,1)	~890
	C-H bend (disubstituted - Z)	~700
	C-H bend (trisubstituted)	~815
alkynes	acetylenic C-H stretch	~3300
	C,C triple bond stretch	~2150
	acetylenic C-H bend	650-600
aromatics	C-H stretch	3020-3000
	C=C stretch	~1600 & ~1475
	C-H bend (mono)	770-730 & 715-685
	C-H bend (ortho)	770-735
	C-H bend (meta)	~880 & ~780 & ~690
	C-H bend (para)	850-800
alcohols	O-H stretch	~3650 or 3400-3300
	C-O stretch	1260-1000

kena ade NH_2
aromatics.

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ethers	C-O-C stretch (dialkyl)	1300-1000
	C-O-C stretch (diaryl)	~1250 & ~1120
aldehydes	C-H aldehyde stretch	~2850 & ~2750
	C=O stretch	~1725
ketones	C=O stretch	~1715
	C-C stretch	1300-1100
carboxylic acids	O-H stretch	3400-2400
	C=O stretch	1730-1700
	C-O stretch	1320-1210
	O-H bend	1440-1400
esters	C=O stretch	1750-1735
	C-C(O)-C stretch (acetates)	1260-1230
	C-C(O)-C stretch (all others)	1210-1160
acid chlorides	C=O stretch	1810-1775
	C-Cl stretch	730-550
anhydrides	C=O stretch	1830-1800&1775-1740
	C-O stretch	1300-900
amines	N-H stretch (1 per N-H bond)	3500-3300
	N-H bend	1640-1500
	C-N Stretch (alkyl)	1200-1025
	C-N Stretch (aryl)	1360-1250
	N-H bend (oop)	~800
amides	N-H stretch	3500-3180
	C=O stretch	1680-1630
	N-H bend	1640-1550
	N-H bend (1^{o})	1570-1515
alkyl halides	C-F stretch	1400-1000
	C-Cl stretch	[illegible]35-540
	C-Br stretch	650-510
	C-I stretch	600-485

nitriles	C,N triple bond stretch	~2250
isocyanates	-N=C=O stretch	~2270
isothiocyanates	-N=C=S stretch	~2125
imines	R_2C=N-R stretch	1690-1640
nitro groups	-NO_2 (aliphatic)	1600-1530&1390-1300
	-NO_2 (aromatic)	1550-1490&1355-1315
mercaptans	S-H stretch	~2550
sulfoxides	S=O stretch	~1050
sulfones	S=O stretch	~1300 & ~1150
sulfonates	S=O stretch	~1350 & ~11750
	S-O stretch	1000-750
phosphines	P-H stretch	2320-2270
	PH bend	1090-810
phosphine oxides	P=O	1210-1140

APPENDIX

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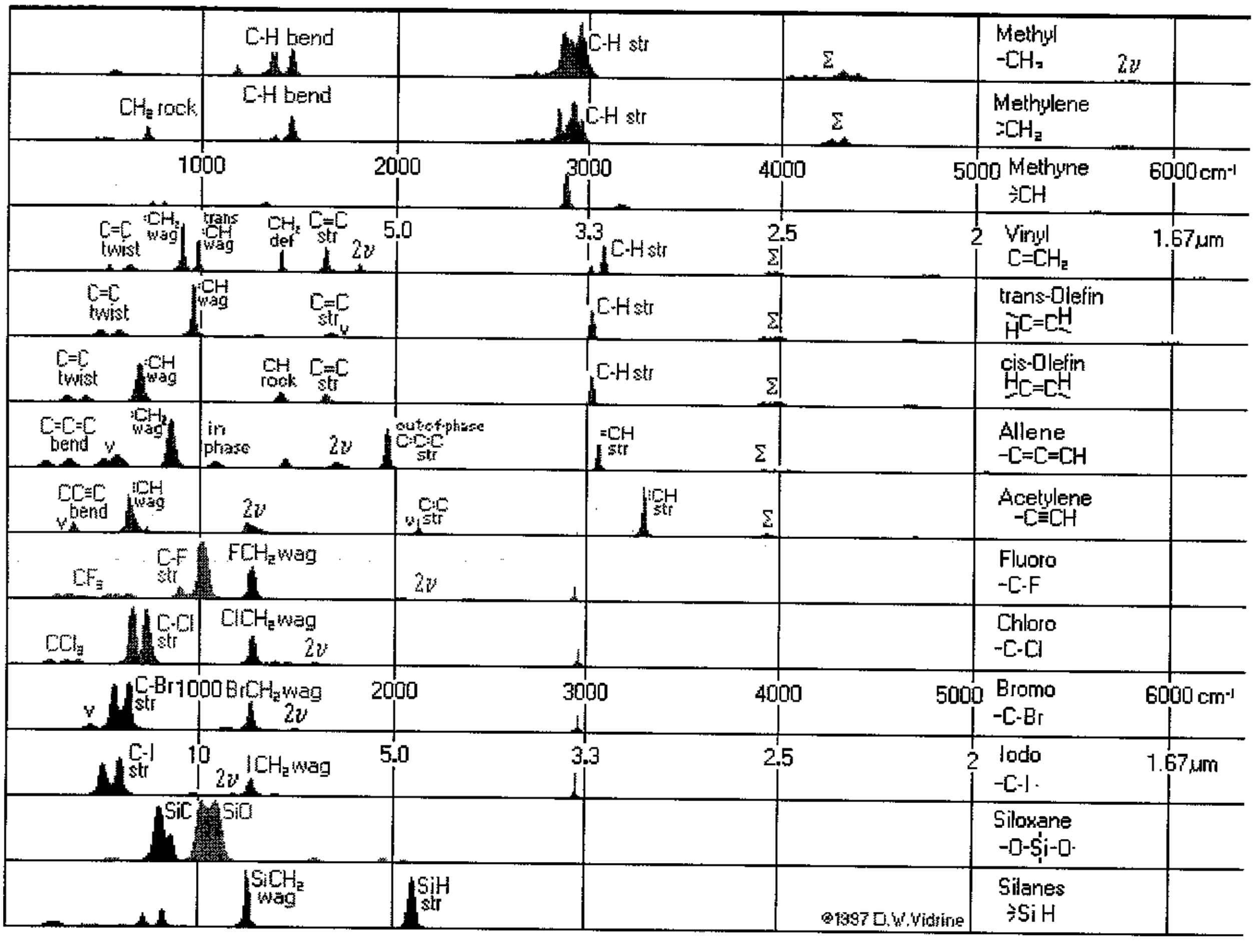
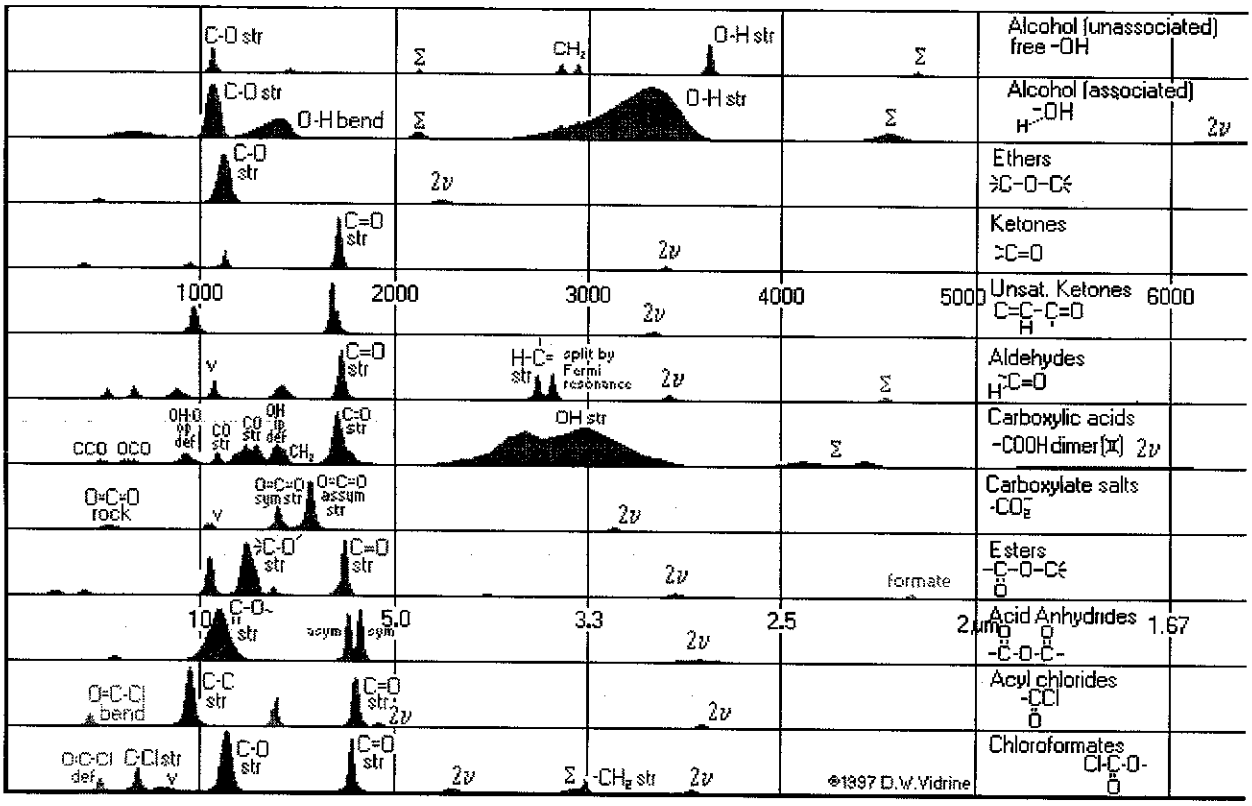
IR CORRELATION TABLES

Aliphatic groups and aliphatic halides



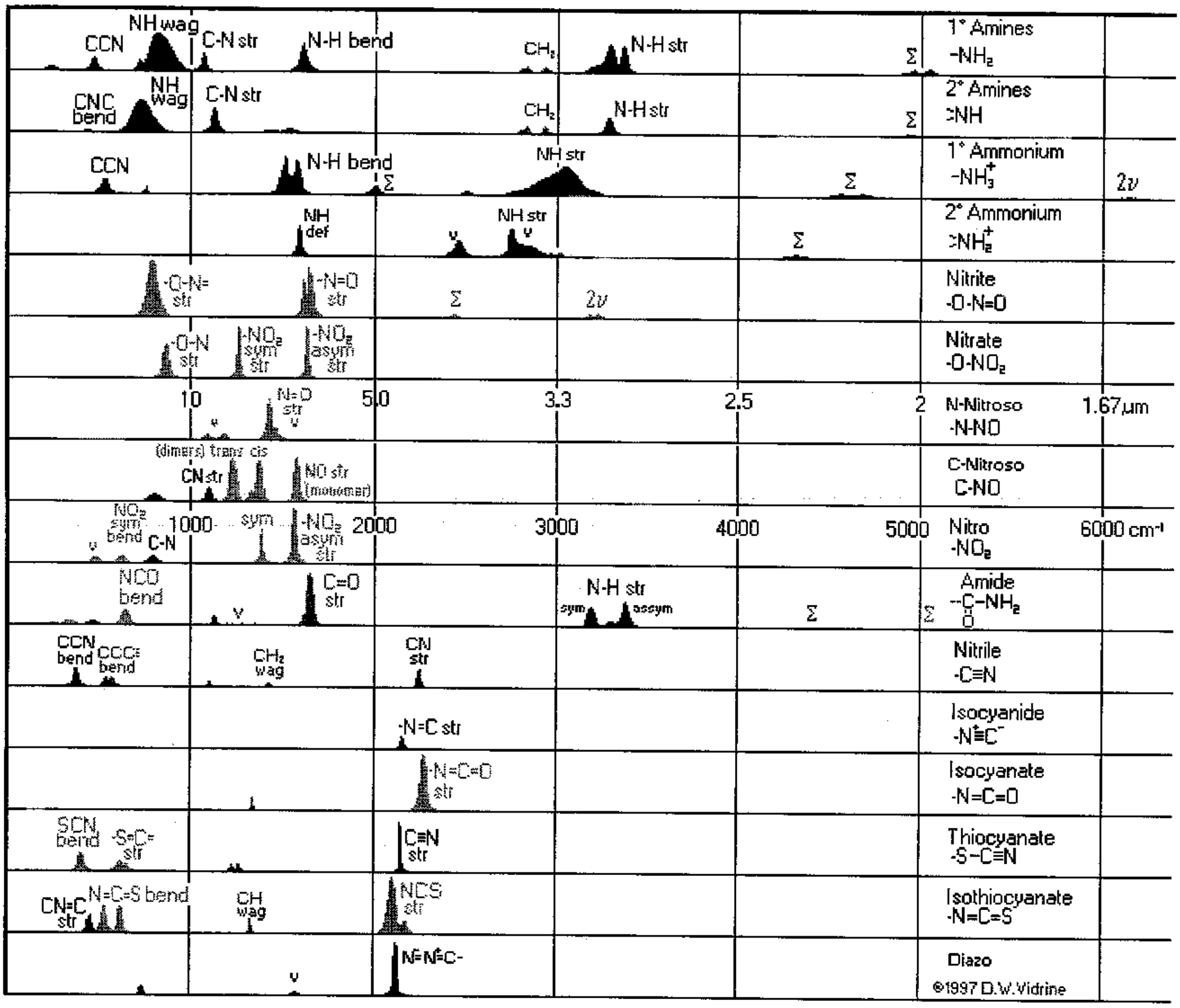
IR CORRELATION TABLES

Functional groups containing oxygen



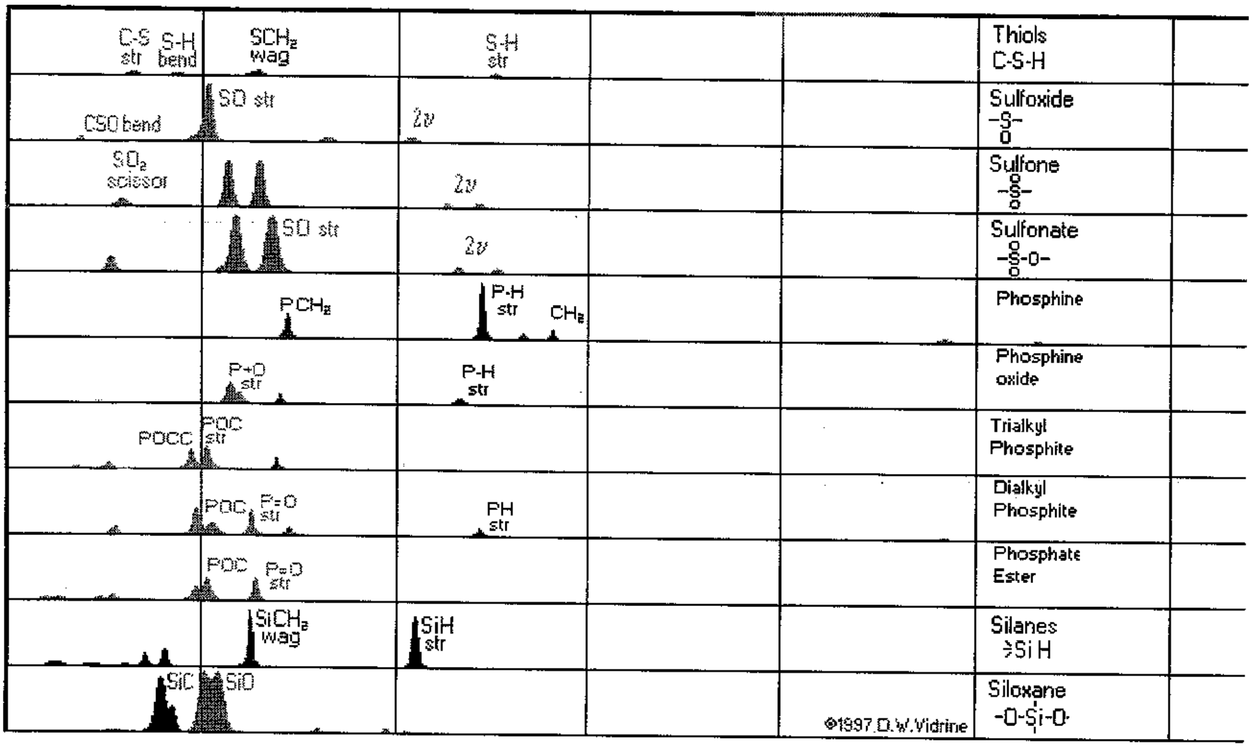
IR CORRELATION TABLES

Functional groups containing nitrogen



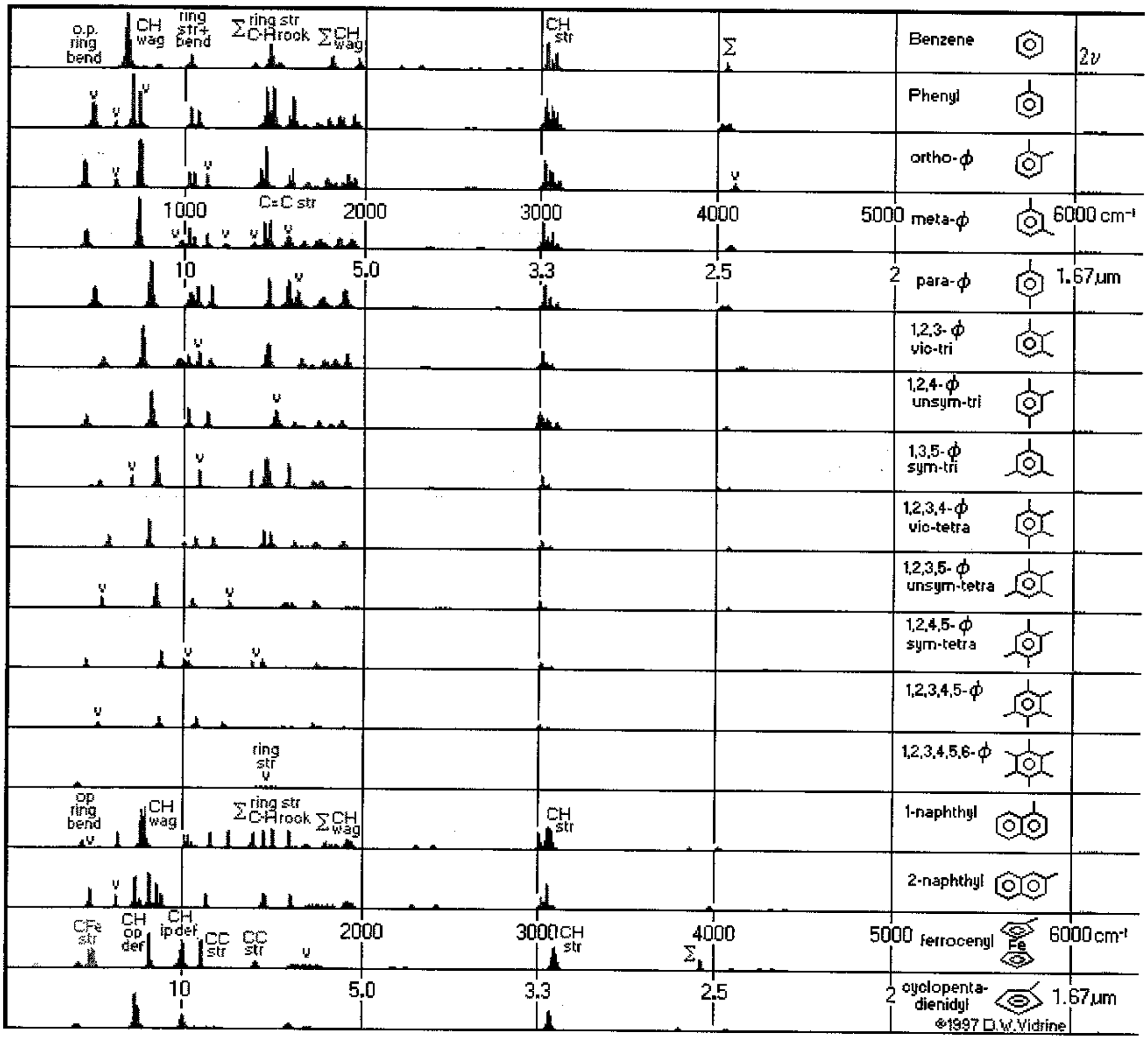
IR CORRELATION TABLES

Functional groups containing sulfur, phosphorus and silicon



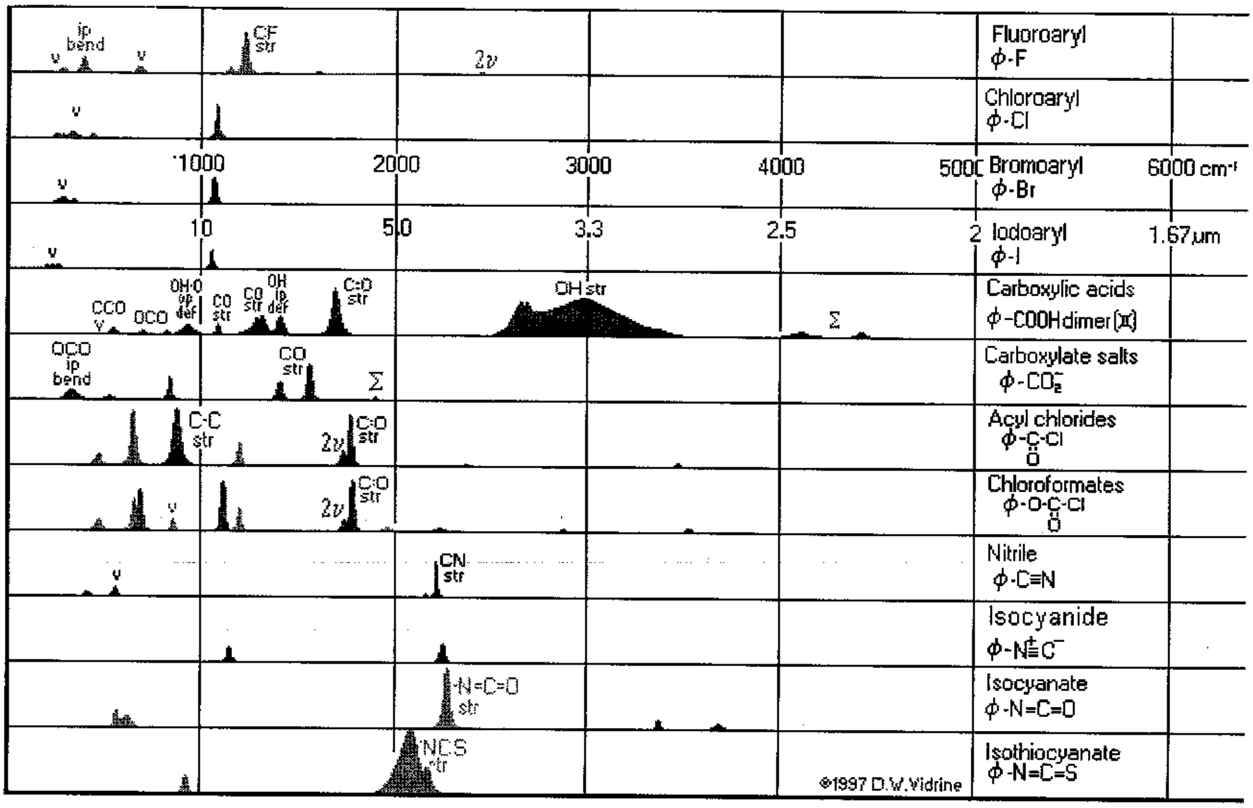
IR CORRELATION TABLES

Aromatic groups



IR CORRELATION TABLES

Functional groups connected to aromatic rings

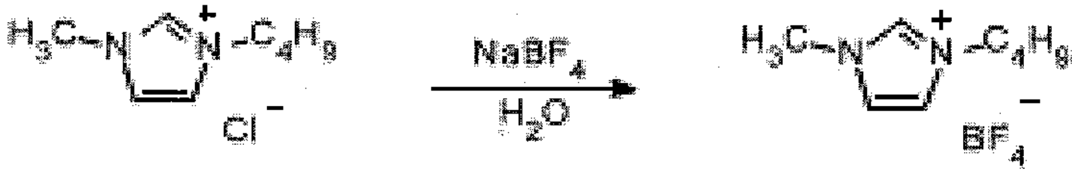


APPENDIX

I

PREPARATION OF 1-BUTYL-3-METHYLIMIDAZOLIUM TETRAFLUOROBORATE

[1H-Imidazolium, 1-butyl-3-methyl, tetrafluoroborate (1−)]



Submitted by Xavier Creary and Elizabeth D. Willis[1].

Checked by Gustavo Moura-Letts and Dennis P. Curran.

1. Procedure

1-Butyl-3-methylimidazolium chloride (30.00 g, 172 mmol) (Note 1) is placed in a 125 mL Erlenmeyer flask containing a stir bar and a thermometer. This salt is dissolved in 35 mL of distilled water and $NaBF_4$ (20.00 g, 182 mmol) (Note 2) is added in portions with stirring over 10-15 min. The $NaBF_4$ dissolves as the mixture emulsifies and cools to 14°C (Note 3). After the mixture warms back to ambient temperature, 30 mL of CH_2Cl_2 is added and the contents are transferred to a 125 mL separatory funnel. The bottom CH_2Cl_2 phase is separated (Note 4). The aqueous phase is extracted with an additional 20 mL of CH_2Cl_2. The combined CH_2Cl_2 phases are shaken in a separatory funnel with a solution of $NaBF_4$ (10.0 g, 91 mmol) in 20 mL of water. The CH_2Cl_2 phase is separated and dried over a mixture of 1.0 g of Na_2SO_4 and 3.0 g of $MgSO_4$. The mixture is filtered through a Büchner funnel and the salts are washed with an additional 15 mL of CH_2Cl_2. A short path distillation head is attached to the 250 mL round-bottom-flask containing the filtrate and most of the CH_2Cl_2 is removed by distillation at 30 mm pressure. Care is taken not to heat the product above 50°C. The solvent is condensed in a receiver flask cooled in an ice-water slurry (Note 5). The last traces of CH_2Cl_2 are removed using a rotary evaporator at 15 mm and 45 °C followed by vacuum drying at ambient temperature until the weight remains constant. The pure 1-butyl-3-methylimidazolium tetrafluoroborate (34.2–34.3 g; 89% yield) is a colorless to pale yellow, viscous liquid (Notes 6-8).

2. Notes

1. The submitters prepared 1-butyl-3-methylimidazolium chloride as previously described.[2] The checkers purchased this from Aldrich Chemical Co.
2. Sodium tetrafluoroborate (98%) was purchased from Acros Organics and used as received.
3. If the emulsion is allowed to stand for 30-60 min, then two phases results. However, there is no need to do this since addition of CH_2Cl_2 induces rapid phase separation.
4. The product at this point is not completely chloride free. In a separate analysis by the submitters, removal of the CH_2Cl_2 from this solution and analysis of 1.53 g of product by titration with 0.100 M $AgNO_3$ (Mohr titration; K_2CrO_4 indicator)[3] required 0.6 mL of the silver nitrate solution to precipitate all of the chloride ion. This corresponds to a product containing 0.7% $BMIM^+$ Cl^- and 99.3% $BMIM^+$ BF_4–.
5. The distilled CH_2Cl_2 has droplets of water from the azeotrope with CH_2Cl_2. This distillation process helps to dry the product and allows recovery of most of the CH_2Cl_2 used in the procedure.
6. Dissolution of 1.50 g of this liquid in 3 mL of water followed by addition of 0.100 M $AgNO_3$ gave no precipitation or cloudiness.
7. The submitters report that the water content of the product was 0.17% as determined from the ^1H NMR spectrum of the neat liquid by integration of the water signal at d 2.9 and the CH_2 signal at d 1.93. The product is hygroscopic and water content increases with exposure to air. The checkers could not detect water in their spectrum in CD_2Cl_2.
8. The product exhibits the following spectroscopic properties: IR (thin film) 3646, 3162, 3122, 2964, 2877, 1575, 1467, 1431, 1171, 1048, 850 cm^{-1}; ^1H NMR pdf (500 MHz, CD_2Cl_2) δ 8.66 (s, 1 H), 7.37 (s, 2 H), 4.14 (t, 2 H, $J = 7.3$ Hz), 3.89 (s, 3 H), 1.81 (quintet, 2 H, $J = 7.4$ Hz), 1.32 (sextet, 2 H, $J = 7.3$ Hz), 0.91 (t, 3 H, $J = 7.3$ Hz); ^{13}C NMR (125 MHz, CD_2Cl_2) δ 136.2, 123.8, 122.5, 49.7, 36.1, 31.9, 19.3, 13.1. Anal. Calcd for $C_8H_{15}BF_4N_2$: C, 42.51; H, 6.69; N, 12.37; Found: C 41.94; H, 6.85; N, 12.37; trace analysis for Cl, 636 ppm.

Waste Disposal Information

All hazardous materials should be handled and disposed of in accordance with "Prudent Practices in the Laboratory"; National Academy Press; Washington, DC, 1995.

3. Discussion

This procedure is based on the general method recently reported in *Organic Syntheses*.[2] The preparation of 1-butyl-3-methylimidazolium hexafluorophosphate ($BMIM^+$ PF_6^-) proceeds as described.[2] However, in our hands, the reported method for the preparation of 1-butyl-3-methylimidazolium tetrafluoroborate ($BMIM^+$ BF_4^-; the most commonly used of the ionic liquids) was not reproducible. The product was contaminated with varying (and significant) amounts of $BMIM^+$ Cl^{-4}. The use of the relatively insoluble KBF_4 (0.44 g/100 mL) in the original preparation makes dissolution and subsequent reaction problematic. Thus, analysis of 0.716 g of a typical ionic liquid product produced from KBF_4 by titration with 0.100 M $AgNO_3$ required 11.1 mL of the silver nitrate solution to precipitate all of the chloride ion. This corresponds to a product containing 27% $BMIM^+$ Cl^- and 73% $BMIM^+$ BF_4^-.

The procedure described herein uses the much more soluble $NaBF_4$ (97.3 g/100 mL). After the first cycle, the chloride content is only 0.7%, and the chloride can no longer be detected after the second cycle. In addition, the tedious process of removing water by distillation under reduced pressure is eliminated. This procedure is also useful for the preparation of the ionic liquid *n*-butyl pyridinium tetrafluoroborate, which is subject to the same chloride contamination problems when prepared from KBF_4. Finally, the amount of residual water in the product can be readily determined from the ^1H NMR spectrum of the neat product.

References and Notes

1. Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN 46556.
2. Dupont, J.; Consorti, C. S.; Suarez, P. A. Z.; de Sousa, R. F. *Organic Syntheses* **2002** *79*, 236.
3. Christian, G. D. “Analytical Chemistry, Fifth Edition”, John Wiley and Sons, Inc., New York, 1994, p. 278.

4. Contamination of $BMIM^+ BF_4^-$ and other ionic liquids with chloride in various preparations has been noted in the literature. See Seddon, K. R.; Stark, A.; Torres, M.-J. *Pure Appl. Chem.* **2000**, *72, 2275.*

Appendix

Chemical Abstracts Nomenclature (Collective Index Number); (Registry Number)

1-Butyl-3-methylimidazolium chloride: 1H-Imidazolium, 1-butyl-3-methyl-, chloride; (79917-90-1)

$NaBF_4$: Borate(1-), tetrafluoro-, sodium; (13755-29-8)

1-Butyl-3-methylimidazolium tetrafluoroborate: 1H-Imidazolium, 1-butyl-3-methyl, tetrafluoroborate (1−); (174501-65-6)

http://www.orgsynth.org/orgsyn/orgsyn/prepContent.asp?prep=v82p0166