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# Properties & Structure of Ionic Liquid

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## Molecular structure of ionic liquid (Z.Meng et al. 2002)

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☞ Non-bonded interaction in ion pairs are of the



exist between

F's on  $\text{PF}_6^-$  and ( 1-butyl-3-methyl imidazolium )

(a) the imidazolium ring N-H

(b) the methyl group H adjacent to the ring

(c) H's on the butyl ( $\text{bmim}^+$ ) side chain

## Molecular structure

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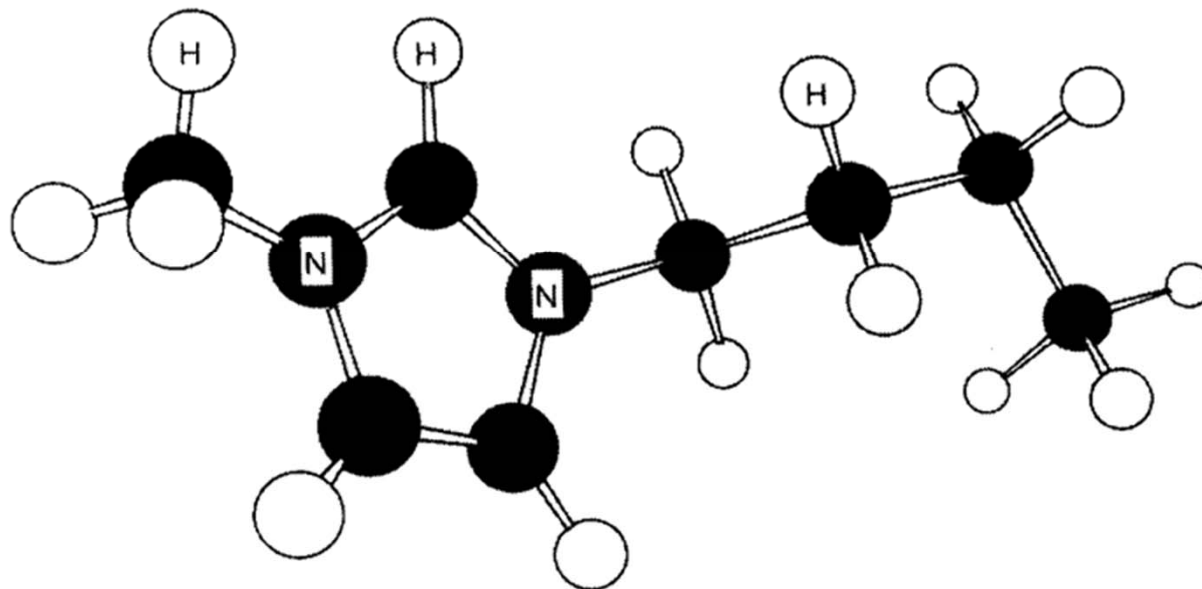
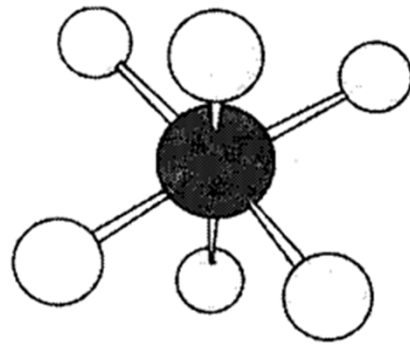
### ☞ Semi-empirical (AM1, PM3) and ab initio structure

- To determine the degree of hydrogen bonding
- To compare the lowest energy models

### ☞ Semi-empirical method

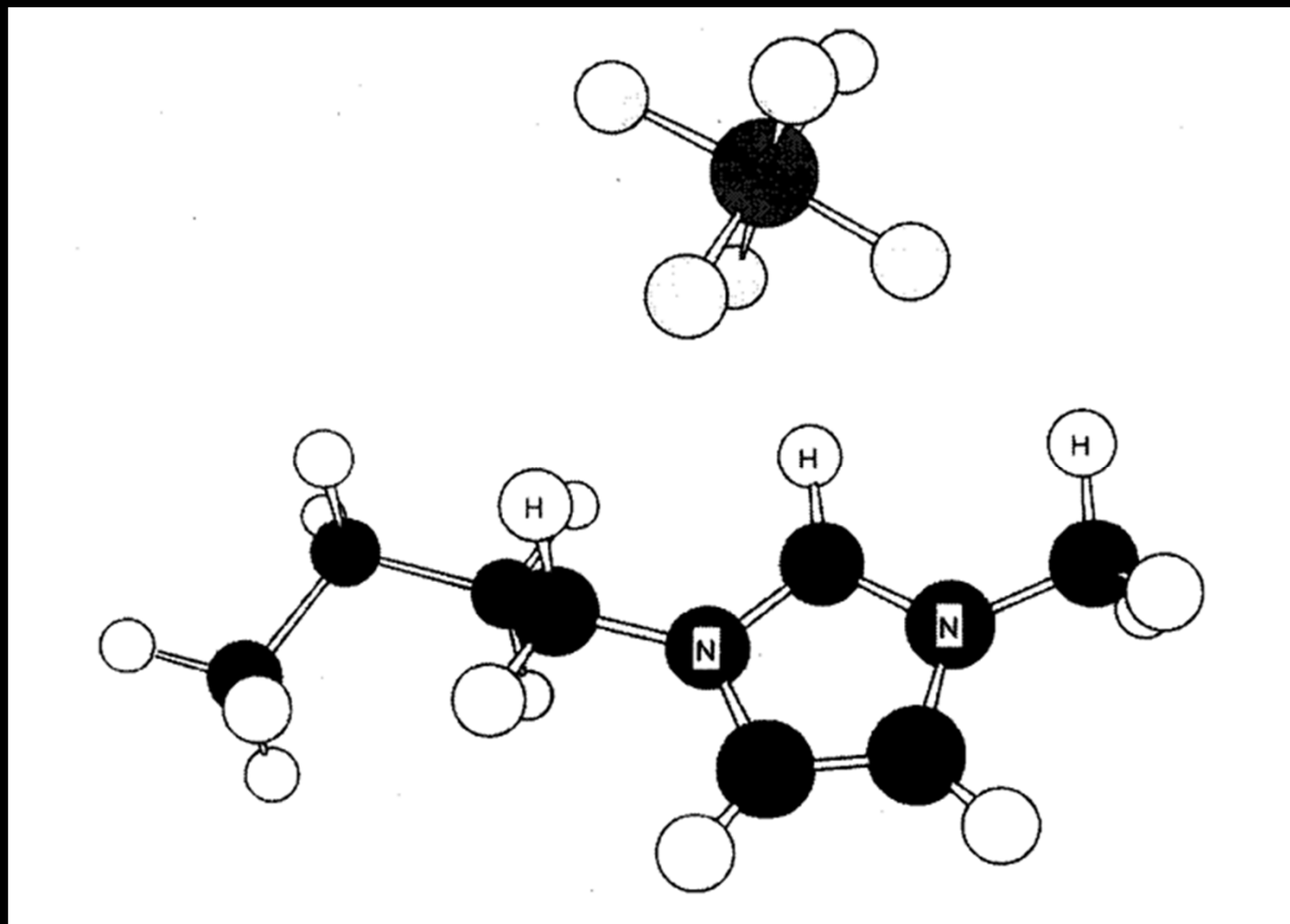
- Minimum energy has AM1, PM3 configuration
- Sites of cation-anion hydrogen bonds
  - Both side chains
  - Above and below the plane of the imidazolium ring
  - Three ring H's
  - Resulted in seven sets of ion pairs

# Molecular structure



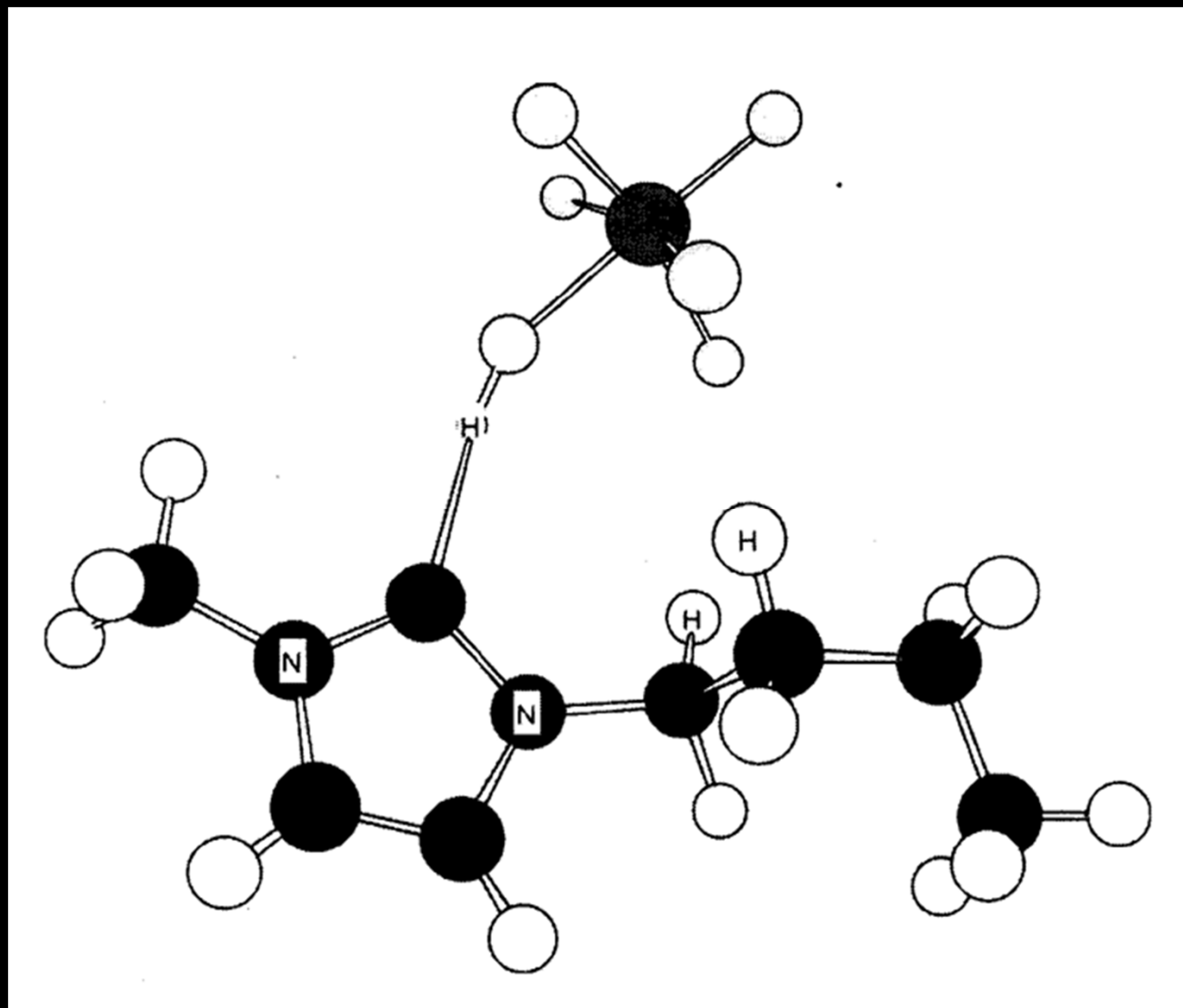
# Molecular structure

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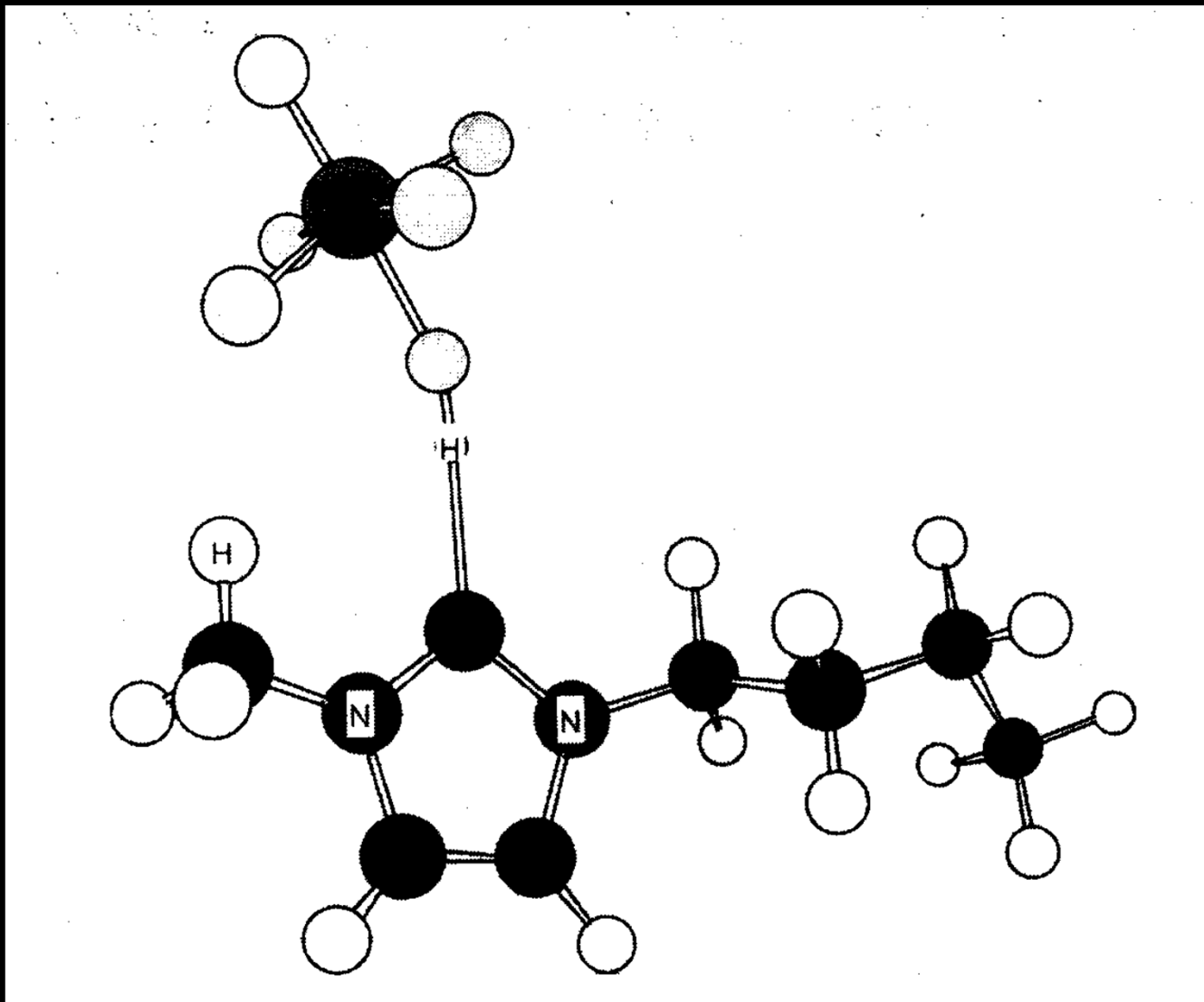
# Molecular structure

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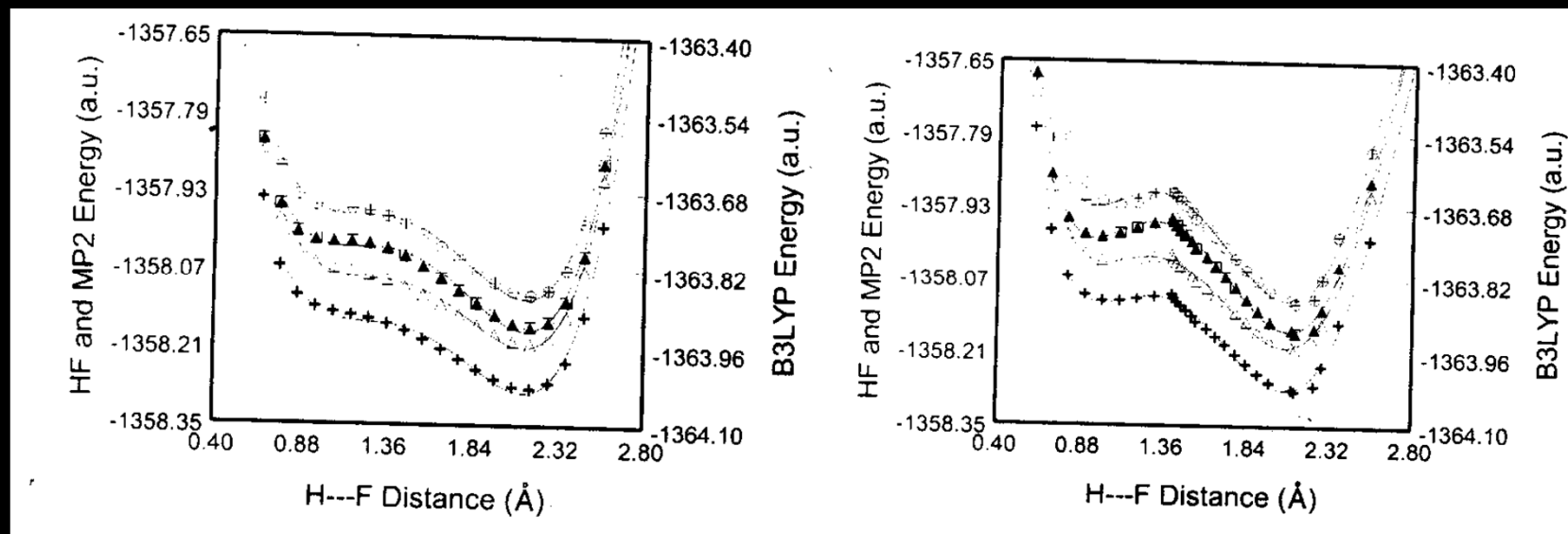
# Molecular structure

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# Molecular structure

## Ab initio structures and energies





# Solubilities of gases in the ionic-liquid

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## ☰ Solubilities at the low pressure

- Gas separation
- Reaction in the ILs as a solvents
  
- 1-n-butyl-3-methylimidazolium hexafluorophosphate
- Carbon dioxide, ethylene, ethane, methane, hydrogen  
carbon monoxide, oxygen, nitrogen, argon
  
- Pressure range : 0 ~ 13 bar
- Temperature : 10, 25, 50 °C

## Solubilities of gases in the ionic-liquid

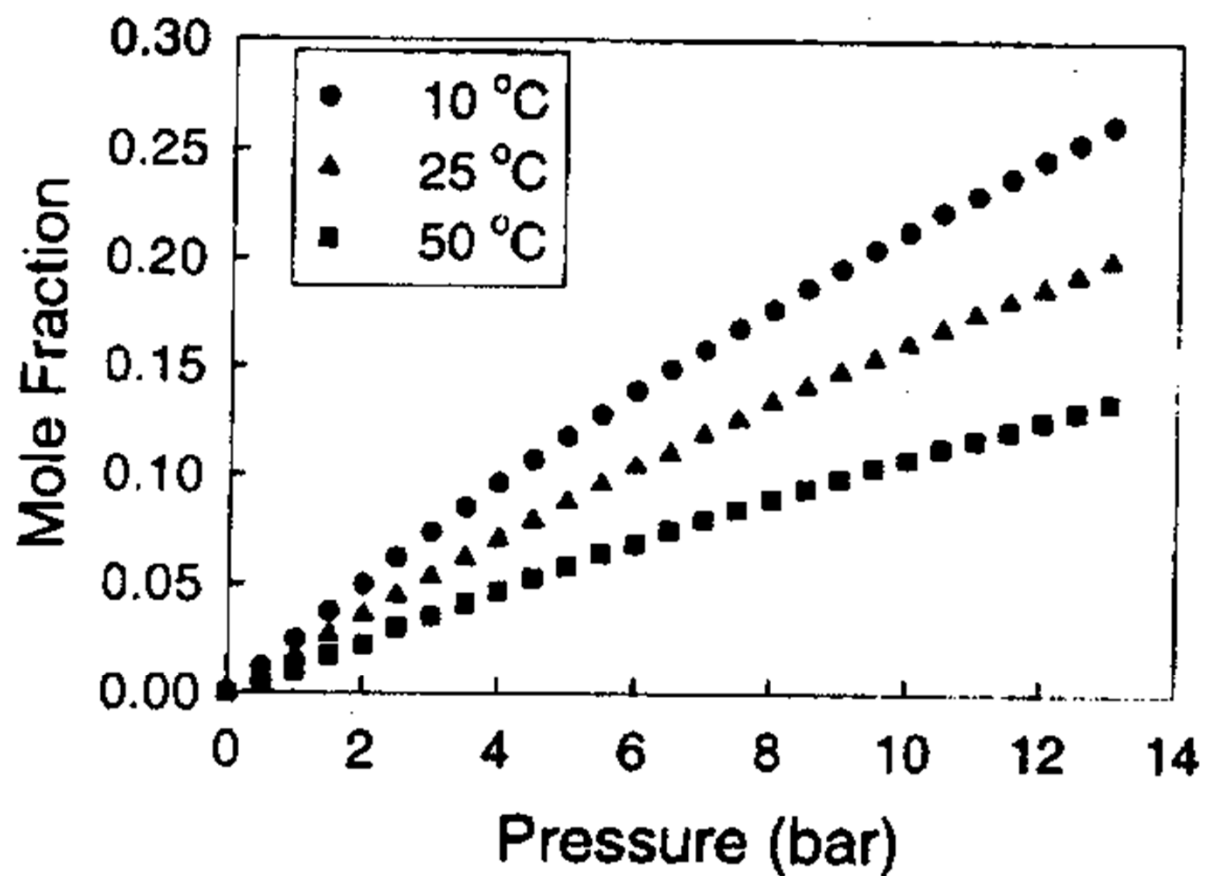


Figure 2. CO<sub>2</sub> solubility in [bmim][PF<sub>6</sub>] at 10, 25, and 50 °C.

## Solubilities of gases in the ionic-liquid

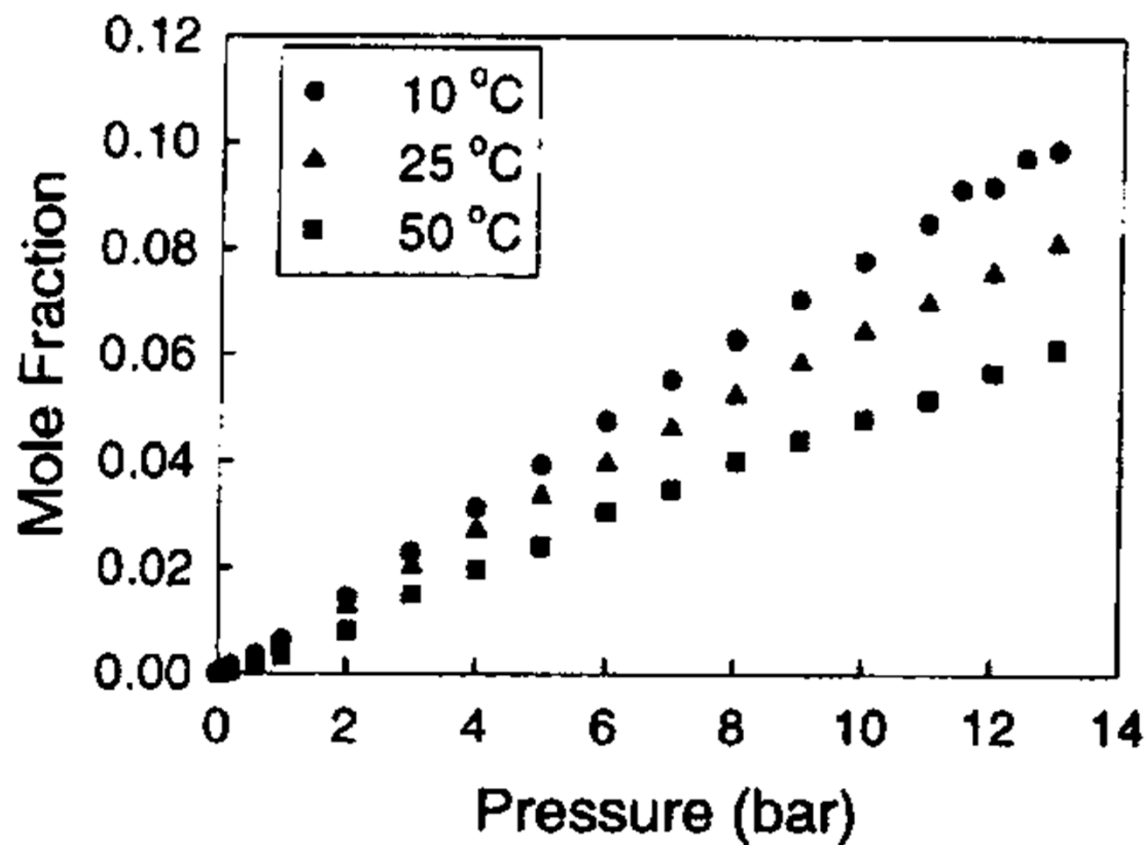


Figure 3.  $C_2H_4$  solubility in  $[bmim][PF_6]$  at 10, 25, and 50 °C.

## Solubilities of gases in the ionic-liquid

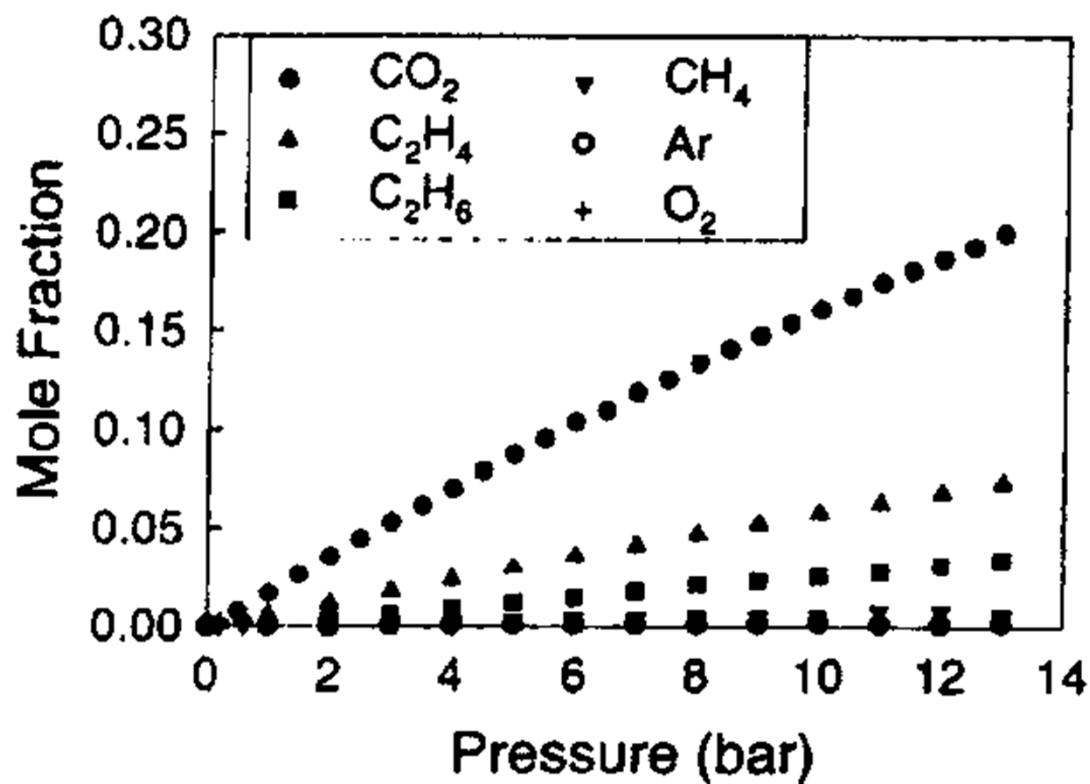


Figure 4. CO<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, CH<sub>4</sub>, Ar, and O<sub>2</sub> solubility in [bmim]-[PF<sub>6</sub>] at 25 °C.

## Effects of Ions

### CO<sub>2</sub> Capture by a Task-Specific Ionic Liquid (Eleanor et al. 2001)

- Interaction between gases and liquid based on separation process
  - Large-scale CO<sub>2</sub> capture is aqueous amines to form ammonium carbamate => loss of capture agent
  - Change the functional group of ionic liquid

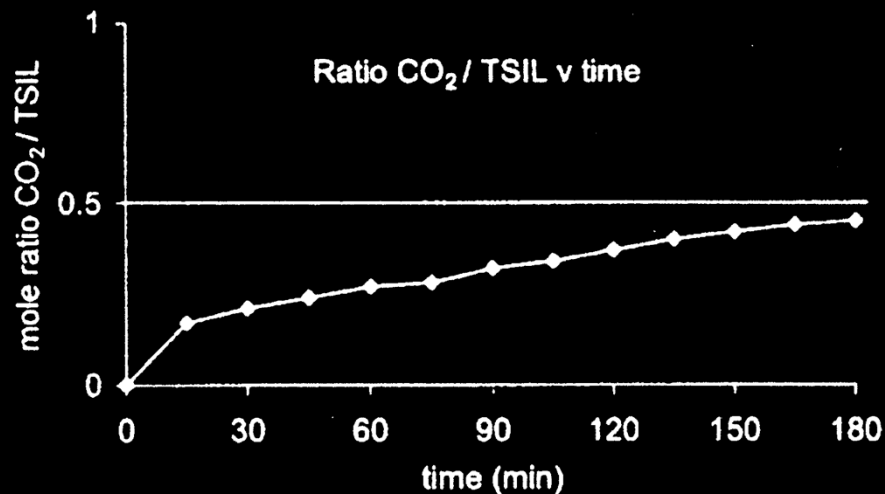


Fig. 4. CO<sub>2</sub>/TSIL molar ratio as a function of time

## References

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- (2) Jennifer L. Anthony; Edward F. Maginn; and Joan F. Brennecke.  
Phys. Chem 2002, 106, 7315
- (3) Eleanor D. Bates; Rebecca D. Mayton; Ioanna Ntai; James H. Davis.  
JACS, 2001, 124, 926