

## Correlation between thermodynamic parameters and spectral characteristics of sorbed CO<sub>2</sub> in ionic liquids studied by *in situ* ATR-FTIR spectroscopy

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Ionic liquids have gained increasing interest because of their outstanding properties over traditional solvents, such as negligible vapour pressures, high thermal and chemical stability, strong solubility capacity, and good recyclability potential. Varying the combination of cations and anions or the chemical functionalities in ILs render an extra degree of freedom to adjust physicochemical properties such as volatility, thermal and chemical stability, solvation, and CO<sub>2</sub> solubility. In turn, the CO<sub>2</sub> molecule exhibits a dual acid-base nature, and can act as both a Lewis acid and a Lewis base<sup>1</sup>. CO<sub>2</sub> has attracted increasing attention as an infrared (IR) probe to monitor the local structure and electrostatic environment or solvation of molecular solvents, because of its sensitivity to chemical and electrostatic characteristics

Fourier transform infrared (FTIR) spectroscopy has proven to be a reliable and robust approach to investigate the interactions between individual solvent, polymers and ionic liquids with CO<sub>2</sub><sup>2-4</sup>. The interaction of CO<sub>2</sub> with homologous series of imidazolium ionic liquids [C<sub>n</sub>MIM][BF<sub>4</sub>] n=2, 4, 6, 8, 10 was studied using *in situ* ATR-FTIR spectroscopy. A systematic investigation into the possible intermolecular interactions of homologous series of ionic liquids with sorbed CO<sub>2</sub> has been carried out. The ionic liquids have been investigated in high-pressure CO<sub>2</sub> environments at increasing temperatures allowing thermodynamic information of the interactions to be determined<sup>5</sup>. A correlation was identified between the enthalpy of dissolution of CO<sub>2</sub> in ionic liquids and the maxima of the positions of the  $\nu_3$  bands of CO<sub>2</sub> (Fig. 1.).

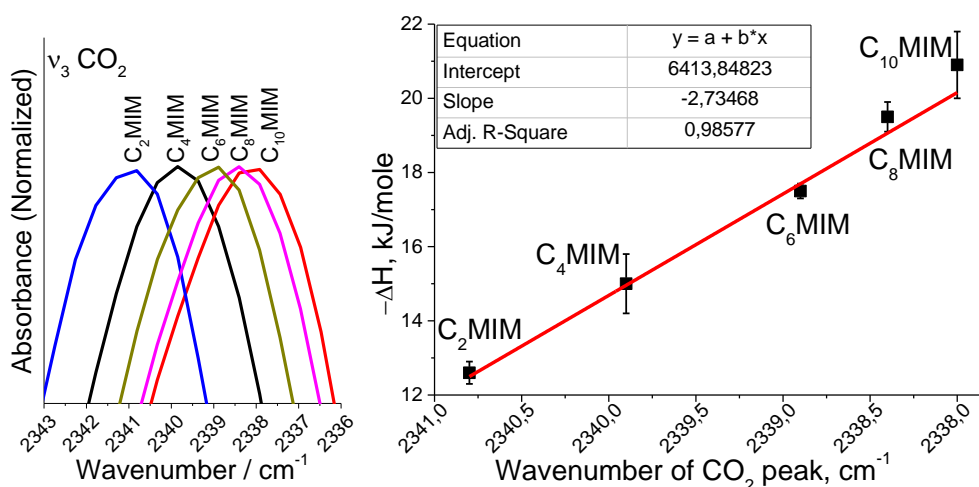


Fig. 1. The average wavenumber of the positions of the  $\nu_3$  bands of CO<sub>2</sub> for different cations and the same [BF<sub>4</sub>] anions in studied ILs. Correlation between enthalpy of dissolution for CO<sub>2</sub> and wavenumber of the  $\nu_3$  bands of CO<sub>2</sub> is presented.

### References

1. Raveendran P. and. Wallen S.L. J. Am. Chem. Soc. 124 (2002) 12590-12599.
2. Kazarian S.G. at al. J. Phys. Chem. 100 (1996) 10837-10848.
3. Kazarian S.G. at al. Chemical Communications. (2000) 2047–2048.
4. Kazarian S.G. at al. Physical Chemistry Chemical Physics. 18 (2016) 6465–6475.
5. Shalygin A.S. at al. Journal of Molecular Liquids. 315 (2020) 113694.

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