

High Pressure CO₂ Absorption Studies on [bmim][PF₆], [bmim][Tf₂N] and [emim][Tf₂N] Ionic Liquids up to 20 MPa: Experimental and Simulation Approach

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In this work we present the high pressure CO₂ absorption performance for common ionic liquids, [bmim][PF₆], [bmim][Tf₂N] and [emim][Tf₂N]. We used high pressure magnetic suspension sorption apparatus for the absorption measurements pressures up to 20 MPa at two different isotherms for each sample. No hysteresis has been observed during the absorption and desorption cycles. Swelling effect at high pressures are corrected and compared with most reliable published data for the same ionic liquids. Moreover, classical molecular dynamics simulations were carried out using the MDynaMix v. 5.0 molecular modelling package. Molecular dynamics were analyzed to infer structural, energetic and dynamic properties of the studied CO₂ + ionic liquids mixed system. Simulations were performed in the NPT ensemble using the Nose–Hoover method to control the temperature and pressure of the simulation system. The equations of motion were solved by Tuckerman–Berne double time step algorithm, with long and short time steps of 1 and 0.1 fs, respectively. The Ewald summation method was implemented for the Coulombic interactions with radius cut-off of 1.5 nm. The simulated systems consist of cubic boxes of pure ionic liquids and ionic liquids with absorbed CO₂ with the compositions reported.