

Guest Gas Enclathration in Tetra-iso-amyl Ammonium Bromide (TiAAB) semiclathrate:  
Thermodynamic and Spectroscopic Approaches

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In this study, tetra-iso-amyl ammonium bromide (TiAAB), one of quaternary ammonium salts, was used for semiclathrate formation. TiAAB forms semiclathrate with water under atmospheric pressure. TiAAB semiclathrate has small vacant cages which can be used for capturing small-sized gas molecules. The large cages of TiAAB semiclathrate are occupied by TiAA cations. TiAAB semiclathrate is most stable at 3.7 mol% which is a stoichiometric concentration. The phase equilibria showed that the TiAAB (3.7 mol%) semiclathrate with CH<sub>4</sub>, N<sub>2</sub>, and CO<sub>2</sub> was significantly stabilized when compared with pure gas hydrate. The enclathration of guest molecules in small cages was confirmed via NMR and in-situ Raman spectroscopy. In addition, the dissociation enthalpy as well as the dissociation equilibrium temperature of TiAAB semiclathrate was measured using a differential scanning calorimeter (DSC). The dissociation enthalpy of pure TiAAB semiclathrate was found to be 214±5.5 kJ/mol·semiclathrate. Through the experimental results obtained in this study, TiAAB semiclathrate is expected to be a potential material for gas storage and separation.