Guest Gas Enclathration in the Tetra-n-butyl Ammonium Chloride (TBAC) Semi-Clathrates: Thermodynamic and Spectroscopic Analyses

김소영, 김연주, 이요한, 김은애, 서용원*
울산과학기술대학교
(ywseo@unist.ac.kr*)

Quaternary ammonium salts (QASs) form semi-clathrate hydrates under higher temperature and lower pressure conditions when compared with the pure hydrate systems. These semi-clathrate hydrates have vacant small cages which can be used for capturing small-sized gas molecules, while the large cages are occupied by the TBA cation. The TBAC semi-clathrate hydrates are expected to have similar properties to the broadly studied QASs such as Tetra-n-butyl ammonium bromide (TBAB) and tetra-n-butyl ammonium fluoride (TBAF). In this study, semi-clathrate phase equilibria of TBAC•29.7H_2O were measured in the presence of various guest gases of CH_4, CO_2, and N_2. The experimental results were compared with TBAB and TBAF. The guest molecules encaged in the semi-clathrate lattices were examined using NMR and Raman spectroscopy. In addition, thermal properties of TBAC were obtained using a differential scanning calorimeter (DSC). The dissociation enthalpy of TBAC•29.7H_2O was found to be 148.6 kJ/mol•semi-clathrate. Through this work, TBAC semi-clathrate hydrates are anticipated for a good candidate as gas storage and separation application.