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Thermodynamic properties of tetra-*n*-butylphosphonium dicarboxylate semiclathrate hydrates

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Abstract (less than 300 words)

Semiclathrate hydrate (SCH) is a crystalline inclusion compounds which consists of host water molecules and guest substances. SCH has been investigated for a thermal storage material by using enthalpy of phase change (around 200 J/g), since the equilibrium temperatures are in the range of 273-300 K. One of the advantages of using SCH is a designability of the thermodynamic properties by selecting the guest substances. Conventional SCHs consists of halide anions, but in recent years, a number of reports on SCHs including monocarboxylate anions from environmental and biocompatibility reasons [1,2] have been reported. In this study, various tetra-*n*-butylphosphonium dicarboxylate (TBP-DC) SCHs in which the dicarboxylate species were oxalate, malonate, succinate, glutarate, maleate, and fumarate, were prepared to investigate the effects of polyvalent ions and steric structures on the thermodynamic and crystallographic properties.

The equilibrium temperatures of TBP-DC SCHs depended on the structure of guest substance, and located in the range of 282.9-290.3 K. The highest equilibrium temperature and the largest dissociation enthalpy, which were observed in TBP-Maleate SCH, were 290.3 K and 206 J/g, respectively. In the presentation, how the dicarboxylate anions affect thermodynamic properties and crystal structure of SCHs will be discussed.

References

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