

이성분계(3차 부틸-히드로과산화물 + 기체) 클러스레이트 하이드레이트의 구조적 특성과 열역학적 안정성에 관한 연구

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Phase equilibria and structure identification of *tert*-butylhydroperoxide + gaseous clathrate hydrates

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Structure-II hydrate has been highlighted due to its higher gas storage capacity and favorable thermodynamic conditions. In this study, we introduce a new structure-II hydrate former, *tert*-butyl hydroperoxide (TBHP) and confirm the structural characteristics through High-Resolution Powder Diffraction (HRPD), ¹³C solid-state NMR and Ramanspectroscopy. Here, we also investigated the thermodynamic stability of binary(TBHP+gaseous) clathrate hydrates. The experimental data were generated using an isochoric pressure-search method. The dissociation data for (TBHP +gaseous) clathrate hydrates are compared with the other hydrocarbon hydrate and pure gaseous hydrate.

Key words : Hydrate(하이드레이트), *tert*-butylhydroperoxide(3차 부틸-히드로과산화물)

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이온성 클러스레이트 하이드레이트의 격자 수축 거동

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Lattice Contraction Behavior Occurring in Ionic Clathrate Hydrate

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Unlike non-ionic clathrate hydrates stably formed by van der Waals interaction between a guest molecule and a surrounding host framework, ionic clathrate hydrates are stabilized by ionic interaction between an ionic guest molecule and the host water-framework. Here, we firstly described the stable entrapment of the superoxide ions in γ -irradiated Me₄NOH + O₂ hydrate. Owing to peculiar direct guest-guest ionic interaction, the lattice structure of γ -irradiated Me₄NOH + O₂ hydrate shows significant change of lattice contraction behavior even at relatively high temperature(120K). Particularly, we note that ionic-induced dimensional change is much greater than thermal-induced change. Such findings are expected to provide useful information for a better understanding of unrevealed nature of clathrate hydrate fields.

Key words : Ionic clathrate hydrate(이온성 클러스레이트 하이드레이트), Superoxide ion(초과산화 이온), γ -irradiation (감마선조사)

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