Structure analysis of propane hydrates

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Clathrate hydrates consist of water cages linked by hydrogen bonds, and various guest molecules. Propane hydrate is contains propane as a guest molecule. The crystal structure is structure II, which is composed of sixteen small cages (S-cage, pentagonal dodecahedron) and eight large cages (L-cage, 16-hedron with 12 pentagonal faces and four hexagonal faces).

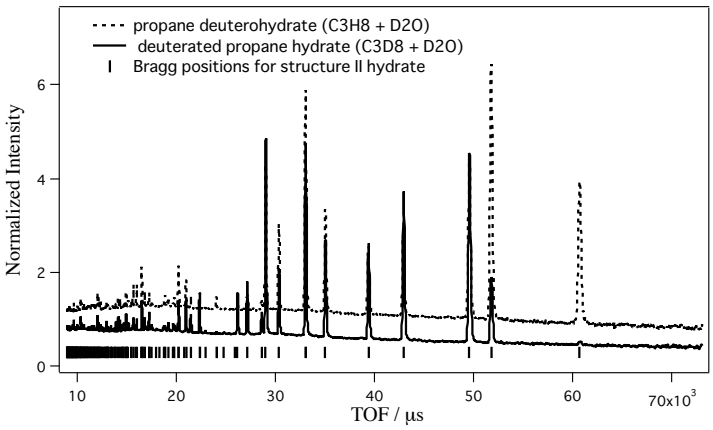

Fig. 1 Comparison of the propane deuterohydrate data with the deuterated propane hydrate data.

We synthesized propane deuterohydrate (C_3H_8 + D_2O) and deuterated propane hydrate (C_3D_8 + D_2O). Powder neutron diffraction data were collected on iMATERIA [1] at MLF. Diffraction data were collected from 10 to 150 K. Figure 1 shows the powder neutron diffraction patterns at 10 K. The diffracted peaks of both C_3H_8 hydrate and C_3D_8 hydrate were almost the same position. However the peak intensities differed between C_3H_8 hydrate and C_3D_8 hydrate. We analyzed by the Rietveld method using Z-Rietveld program [2]. Neutron diffraction patterns revealed that our samples were crystallized as structure II hydrate. We will compare with the previous results [3] and will discuss the difference from our results and temperature dependence of the crystal structure.

References

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