NEUTRON POWDER DIFFRACTION STUDY OF TYPES I & II TRIMETHYLENE OXIDE HYDRATES AS A FUNCTION OF TEMPERATURE

A.J. Rondinone[1], Y. Ishii[2], B.C. Chakoumakos[1], C. J. Rawn[1], and S.L. Marshal1[1]
[1]Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA 37831
[2]Japan Atomic Energy Research Institute, Tokai, Ibaraki, Japan

Trimethylene oxide (TMO) is of interest because it forms type I or type II hydrates depending on stoichiometry. The structures of types I & II TMO hydrates were synthesized from D_2O and hydrogenated TMO at the ratio of 6.25:1 D_2O:TMO for the type I and 17:1 D_2O:TMO for the type II. The samples were studied with powder neutron diffraction at the JAERI High Resolution Powder Diffractometer (JRR-3M). The guest-host interaction of TMO in the large cavities was modeled using a rigid body approximation of the gas phase TMO molecule. Data were collected at 10, 40, 70, 100, 130, 160, 190, 220, and 250K for both crystal structures. The atomic displacement parameters were used to compare guest-host interactions of the types I & II hydrates. The temperature dependencies of the lattice constants were used to calculate thermal expansivities.

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