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Dynamics of trimethylene oxide in a structure II clathrate hydrate

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ABSTRACT

Neutron scattering has been used to study the dynamics of trimethylene oxide (TMO) in a structure II clathrate hydrate. Two regimes of guest dynamics have been identified in the range 10 K to 100 K. Below 50 K, the hydrogen atoms on TMO execute jumps between nonequivalent sites with a jump distance of 2.1 Å, consistent with a model of rotations of 90° about the C_{2v} molecular axis between sites with unequal occupancy probabilities, and corresponding to an energy difference between sites of ~7 meV. Above 50 K, a second dynamical regime appears in which rotational motions of H occur about both the C_{2v} axis and a second axis perpendicular to the plane of the molecule. An increase in the activation energy barrier to the motion that appears to accompany the onset of multi-axis motion could be a result of the additional high-energy rotations taking place within more restricted cross-sections of the cage.