

Raman spectroscopic studies of phase E to 19 GPa

ANNETTE K. KLEPPE,^{1,*} ANDREW P. JEPHCOAT,^{1,†} AND NANCY L. ROSS²

¹Department of Earth Sciences, University of Oxford, Parks Road, Oxford OX1 3PR, U.K.

²Department of Geological Sciences, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061, U.S.A.

ABSTRACT

Raman spectra of phase E have been measured between 100 cm⁻¹ and 4000 cm⁻¹ in a diamond-anvil cell to 19 GPa at 300 K. We observe several broad bands in the region below 1200 cm⁻¹ and three bands in the OH stretching region. All modes shift continuously with increasing pressures to 19 GPa and there is no indication for a major change in the crystal structure of phase E. First constraints on hydrogen sites and hydrogen bond strengths are derived from the OH frequencies together with their pressure dependencies and the correlation of OH stretching frequencies with O···O bond distances. The 3429 cm⁻¹ band decreases linearly with pressure at -7.8 cm⁻¹/GPa and is clearly involved in hydrogen bonding. The corresponding O···O distance at ambient conditions is estimated to be around 2.82 Å. The 3617 cm⁻¹ band shows a positive pressure trend allowing only very weak or absent hydrogen bonds. Corresponding O···O distances would be greater than 3 Å.