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**Molecular dynamics for Raman modes of high pressure phases of hydrogen** IOAN-BOGDAN MAGDAU, GRAEME JOHN ACKLAND, CSEC, University of Edinburgh — We present ab initio molecular dynamics (MD) calculations of hydrogen at high temperature. We calculated the Raman spectra for phases III and IV and make direct comparison of Raman vibrons with experiment. The MD structures are sensitive to initial conditions and system size, but experimental comparison provides excellent discrimination between structures found, and enables us to explain some of the existing anomalies in the literature. Structures observed for pressure-temperature conditions of phase IV are based on layers of ordered molecules and layers of either static or freely rotating hexagonal trimers, however only two are consistent with experiment. The high temperature phase IV is a hexagonal structure with alternate layers of freely rotating hydrogen molecules, and hexagonal trimers. The low temperature phase III is similar to the C2/c structure previously proposed. These structures are qualitatively different from previous work which introduced spurious features through finite size effects. The MD properly accounts for anharmonic effects and gives much better agreement with Raman data than lattice dynamics calculation.

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