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Hydrogen bonding and coordination in normal and supercritical water from X-ray inelastic scattering P. H.-L. SIT, DMSE, MIT, CHRISTOPHE BELLIN, Institut de Minèralogie et de Physique des Milieux Condensès, Universitè Pierre et Marie Curie, BERNARDO BARBIELLINI, Department of Physics, Northeastern University, D. TESTEMALE, J.-L. HAZEMANN, Laboratoire de Cristallographie, CNRS, T. BUSLAPS, European Synchrotron Radiation Facility, NICOLA MARZARI, DMSE, MIT, ABHAY SHUKLA, Institut de Minèralogie et de Physique des Milieux Condensès, Universitè Pierre et Marie Curie
— A direct measure of hydrogen bonding in water under conditions ranging from the normal state to the supercritical regime is derived from the Compton scattering of inelastically-scattered X-rays. First, we show that a measure of the number of electrons n_e involved in hydrogen bonding at varying thermodynamic conditions can be directly obtained from Compton profile differences. Then, we use first-principles simulations to provide a connection between n_e and well-defined structural measures for the number of hydrogen bonds n_{HB}. Our study shows that over the broad range studied the relationship between n_e and n_{HB} is linear, allowing for a direct experimental measure of bonding and coordination in water. In particular, the transition to supercritical state is characterized by a sharp increase in the number of water monomers, but also by a significant number of residual dimers and trimers.

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