Hydrogen bonding and coordination in normal and supercritical water from X-ray inelastic scattering P. H.-L. SIT, DMSE, MIT, CHRISTOPHE BELLIN, Institut de Minéralogie et de Physique des Milieux Condensés, Université 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 Minéralogie et de Physique des Milieux Condensés, Université 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.