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Pseudo-spin model and neutron scattering studies of hydrogen disorder in D_2O DAVID JONATHAN P. MORRIS, Xavier University, Cincinnati, OH, USA, KONRAD SIEMENSMEYER, BASTIAN KLEMKE, JENS-UWE HOFFMANN, ILLIA GLAVATSKYI, KLAUS SEIFERT, Helmholtz-Zentrum Berlin for Materials and Energy, Berlin, Germany, SERGEI ISAKOV, ETH Zurich, Switzerland, RODERICH MOESSNER, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany, ALAN TENNANT, Oak Ridge National Laboratory, Oak Ridge, TN, USA — The crystal structure of water is made up of a regular lattice of oxygen atoms connected by hydrogen bonds with an intermediate hydrogen atom. The hydrogen atom is displaced from the midpoint between nearest neighbor oxygen-oxygen atoms. Therefore the H-bond between neighboring hydrogen and oxygen can either be short or long. These H-bonds are known to obey the famous "ice rules" where each oxygen has two neighboring hydrogen sitting on the close site and two neighboring hydrogen sitting on the further site. The ice rules do not specify which hydrogen bonds will be short and which will be long for any particular oxygen, i.e. they do not describe long-range order, merely that there will be two short and two long bonds for a particular oxygen atom allowing for disorder. Here we will present a pseudo-spin model of water ice and diffuse neutron scattering measurements from D_2O. The displacements of hydrogen away from the midpoint between neighboring oxygen-oxygen are treated as interacting Ising spins ($\sigma = \pm 1$). The diffuse neutron scattering measurements allow us to test the resulting theoretical predictions.

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