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Interplay Between Local Structure and Nuclear Dynamics in Tungstic Acid: a Neutron Scattering Study

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We provide an exhaustive characterization of structural properties and nuclear dynamics in tungstic acid (WO3·H2O). To this end, we employ Neutron and X-ray Diffraction (ND and XRD) combined with Inelastic Neutron Scattering (INS) and Neutron Compton Scattering (NCS) experiments, and corroborate the analysis with extensive ab initio modelling. The first step in our analysis is the elucidation of the crystal structure based on the refinement of low-temperature powder ND data, extending the knowledge gained from XRD analysis of a mineral specimen of tungstite. These results are confronted with low-temperature INS experiments and zero-temperature phonon calculations. The analysis reveals an inconsistency in the definition of the structure of confined water with respect to crystallographic data, also showing a concomitant fail of the phonon calculations due to a strongly anharmonic confining potential. Extending the computational route toward ab initio MD (AIMD) simulations allows us to probe different structural configurations and provides an improved description of the vibrational dynamics as compared to high-resolution INS experiments, nevertheless, requiring the use of effective classical temperatures. The analysis of both INS and the NCS data reveals a remarkable similarity to the nuclear dynamics earlier reported for water confined in Single-Wall Carbon Nanotubes (SWNT), which has been qualitatively described as a new phase of ice. Our analysis reveals a strong two-dimensional hydrogen-bonding network, similar to the shell model for water in SWNT. The reported NCS data show narrowing of the hydrogen momentum distribution with respect to the reference ab initio calculations, indicating a great deal of conformational freedom due to spatial delocalisation of protons in the ground state of the system, a clear signature of the quantum character of the nuclei.

Primary authors: Dr MATTHEW, Krzystyniak (ISIS Neutron Spallation Source, RAL, UK); Dr DRUZBICKI, Kacper (Polish Academy of Sciences, Lodz, Poland); Dr ERWIN, Lalik (Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences); Dr GAVIN , Irvine (School of Chemistry, University of St Andrews, St Andrews, Fife KY16 9ST, United Kingdom); Dr GUTMANN, Matthias (ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, United Kingdom); Dr RUDIC, Svemir (ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, United Kingdom); Dr MANUEL, Pascal (ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, United Kingdom); Dr VACLAV , Petricek (Institute of Physics, Czech Academy of Sciences, Na Slovance 1999/2, Praha 8, 182 21, Czech Republic)

Presenter: Dr MATTHEW, Krzystyniak (ISIS Neutron Spallation Source, RAL, UK)

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