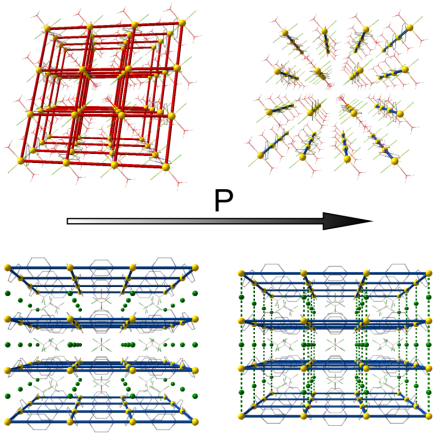

Figure 1. High pressure can alter the dimensionality of the magnetic exchange in Cu-pyz based quantum magnets. Thick lines represent magnetic exchange pathways and different colours indicate H-bonds-, pyz- or X- mediated interactions, (in red, blue and green, respectively).

Keywords: high-pressure, quantum magnets, spin density

MS23-O4 Hydrogen maleate salts: Precise and accurate determination of the hydrogen atom position in short hydrogen bonds using X-ray diffraction at extremely low temperatures

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Hydrogen maleate salts offer the unique opportunity to follow a pseudo-reaction pathway of a proton transfer not only in theoretical simulations but also experimentally because the hydrogen position in the strong and short intramolecular O-H-O hydrogen bond is highly flexible dependent on the cation. There are numerous crystal structures of hydrogen maleate salts in the literature showing that the O-O distance is constant around 2.45 A, but the O-H distances vary from 0.83 A/1.63 A in highly asymmetric hydrogen bonds to 1.22A in symmetric hydrogen bonds with a large variety of intermediate distances. This means that snapshots along a pseudo-reaction pathway can be measured and with the symmetric hydrogen bonds, even a model for a possible transition state is accessible. Experimental electron-density modelling of high-resolution low-temperature (20K) synchrotron X-ray data of nine different compounds (4-aminopyridinium, 8-hydroxyquinolinium, barium, calcium, potassium, lithium, magnesium, sodium and phenylalaninium hydrogen maleates) measured at SPring-8, Japan, will give electronic information on the pseudo-reaction mechanism.

For these detailed electron-density analyses, it is crucial to obtain accurate positional and displacement parameters of the hydrogen atoms. It is a widespread notion that this can only be achieved using neutron-diffraction techniques. Therefore we have collected Laue-diffraction neutron data at the Bragg institute of ANSTO, Australia. Using those data as a reference, we will show that we can obtain hydrogen atom positions and bond lengths involving hydrogen atoms with the same accuracy and precision from X-ray data as from neutron data - even from X-ray data of routinely achievable resolution - if an advanced X-ray refinement technique is used. This new technique is called Hirshfeld Atom Refinement (HAR) [1].

[1] S. C. Capelli, H.-B. Bürgi, B. Dittrich, S. Grabowsky, D. Jayatilaka: Hirshfeld atom refinement. IUCrJ 2014, 1, 361-379.

Keywords: hydrogen maleate salts, Hirshfeld atom refinement, hydrogen atom parameters from X-ray diffraction