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A pedagogical journey in search of hydrogen disorder with RMCProfile analysis of X+n data from hydrogrossular

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The structure of fully hydrated grossular, Ca3Al2[(OH)4]3, contains an unusual arrangement of four O-H bonds within each tetrahedral cavity when all SiO4 in the anhydrous form are substituted for (OH)4. Neutron and x-ray total scattering from a powdered deuterated sample were measured and modelled using RMCProfile to investigate the local arrangement of this O4D4 cluster [1]. This showed that, other than the consequences of a correctly determined (and longer) O-D bond length, there is little to suggest that the O4D4 structure is locally significantly different from that expected based on the average structure determined solely from Bragg diffraction.

This talk will therefore concentrate on the X+n total scattering data analysis process, which proved very instructive, provided a few surprises, and will hopefully be of help to others using total scattering/PDF data to understand disorder in crystalline materials.

[1] D A Keen, D S Keeble and T D Bennett. Phys. Chem. Miner. 45 (2018) 333-342

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