Poster Presentation

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Neutron Diffraction Investigation on the Symmetrical Hydrogen Bond in K3H(SO4)2

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In this work, we present a structure investigation on K3H(SO4)2 by single crystal neutron diffraction. Letovicite with a chemical composition (NH4)3H(SO4)2 belongs to a large family of M3(H,D)(XO4)2 compounds, where M = K+, Rb+, (NH4)+, Cs+, Tl+ and X = Se6+ and S6+. This compound crystallizes in the monoclinic space group A2/a with a = 9.789(7) Å, b = 5.6815(9) Å, c = 14.703(2) Å and β = 103.03(4)° at 300K. At 2.3K, the lattice parameters are a = 9.687(20) Å, b = 5.648(13) Å, c = 14.613(9) Å and β = 103.23(14)°. Data at 2.3K were measured up to (sinθ/λ) = 0.807Å-1 with the single crystal neutron diffractormeter HEiDi at the FRM-II, Germany. H/D shows a dynamic disorder at high temperature, which can be related to very high proton conductivity. In letovicite, two types of disorder related with hydrogen atoms are reported [1]. Although letovicite shows various phase transitions owing to the proton ordering at low temperature, K3H(SO4)2, without the possibility of an orientational disorder of NH4+, undergoes no phase transition at low temperature. At room temperature, the title compound is isostructural to lectovicite, and has an inversion center in the middle of the SO4-H-SO4 dimer. The bond length, 2.483(3) Å, and bond angle, 180°, support the hypothesis that the disordered proton shows a double-well potential, if the distance between the oxygen atoms of the hydrogen bond Ro-o are longer than a critical bond length rc(2.47 Å for protons and 2.40 Å for deuterons) [2]. However, it is not easy to determine if the hydrogen bond is a low-barrier hydrogen bond (LBHB) or centered hydrogen bond (centered HB). Based on an analysis of the anisotropic parameters, the bond lengths and elongation of the hydrogen atom toward the two oxygen atoms by neutron single crystal diffraction experiments at 300K and 2.3K, it seems that the hydrogen bond in the title compound can be classified as a centered hydrogen bond or intermediate form between a cigar-like shape and the disk-like shape [3].

[1] *Y. Sohn, Doctoral Thesis, RWTH Aachen, 2012,* ***[2]*** *Y. Noda, H. Kasatani, Y. Watanabe, and H. Terauchi, Journal of the Physical Society of Japan 1992, 61, 905.,* ***[3]*** *M. Benoit, and D. Marx, ChemPhysChem, 2005, 6, 1738.*

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