Charge Ordering and Magnetic Structure in Fe_3BO_5

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The structure of $(Fe^{2+})_2(Fe^{3+})O_2BO_3$ ludwigite (space group Pbam, a=9.462A, b=12.308A, c=3.075A) is made of zigzag walls of edge-sharing FeO_6 octahedra, connected by BO_3 triangular groups. It contains two types of 3-leg ladders of Fe cations: ladder 1 with only Fe^{2+} cations and ladder 2 formed by Fe^{3+} cations with one additional electron per rung delocalized at high temperature. This leads to a quite complex physical behavior. Two magnetic ordering transitions are observed at 112K and 70K. Specific heat shows a plateau between ≈100K and 250K, and a change of slope of resistivity is observed close to room temperature. Using single crystal x-ray diffraction, we have shown that it is due to a partial localization of the Fe 3d electrons on ladder 2, accompanied by a superstructure doubling the c-axis.

We report here the investigation of the magnetic ordering, using neutron powder diffraction on I.L.L. D20 between 300K and 10K. Based on the superstructure found with x-rays, both magnetic structures were solved and refined by the Rietveld technique. Between 70K and 110K, only ladder 2 is ordered. The coupling is ferromagnetic in the rungs and antiferromagnetic between them. At 70K, ladder 1 orders as a canted antiferromagnet in the rungs which are ferromagnetically coupled. This also leads to a partial reorientation of the spins of ladder 2. A strong magnetic background increasing from room temperature to 110K could be related to short range correlations in both magnetic sub-units.

Keywords: magnetic structure determination, superstructure, spin ladder