Poster Presentation

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Synthesis and crystal structure of a new layered $CoBi_2O_2F_4$ oxofluoride

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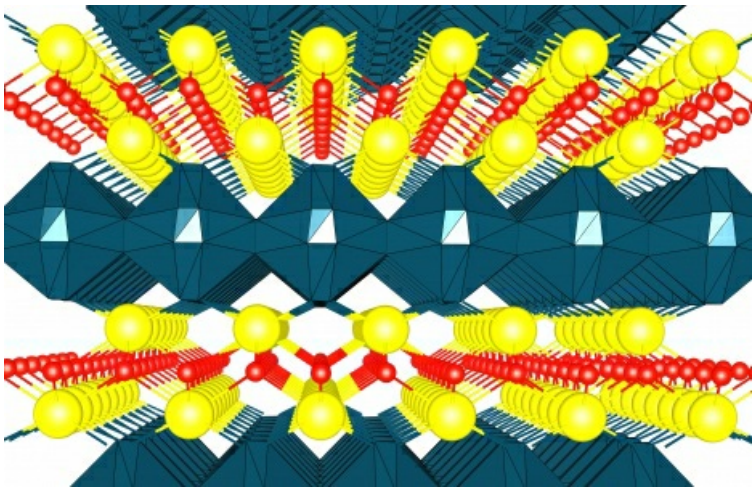
Single crystals of the new oxo-fluoride CoBi2O2F4 were successfully grown by a hydrothermal technique at 200ºC. The crystal structure was solved from single crystal X-ray diffraction data, collected at different temperatures; 100 K, 298 K, 243 K and 293 K. The compound is layered and crystallizes in the tetragonal non-centrosymmetric space group I-4 where a=3.843(2) Å, c=16.34(8) Å. Two building blocks make up the crystal structure; [BiO4F4] distorted cubes and distorted [CoF6] octahedra. Interestingly the F atoms of [CoF6] show four-fold splitting at room temperature. The disorder of the F atoms is temperature dependent and decreases with decreasing temperature. The [CoF6] octahedra are connected to each other via corner sharing to form [CoF4]∞ layers. In between there are layers of [BiO4F4] polyhedra connected by Bi – O bonds to form [BiO2F2]∞ layers where the F-atoms further connect to the [CoF4]∞ layers. Raman scattering data were collected at various temperatures from room temperature to 10 K in order to investigate the disorder in the structure. Sharper phonon peaks appeared and several modes revealed as the temperature decreases which is an indication of reduction in structural disorder. Magnetic susceptibility and heat capacity measurements showed long range anti-ferromagnetic ordering below the Néel temperature of ~50 K. The magnetic susceptibility follows the Curie-Weiss law above 75 K with the Curie Weiss temperature θ = -100 K, the Curie constant C = 3.53 emu·K·mol-1 and the effective magnetic moment μeff = 4.34 μB.



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