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Magnetic quadrupolar order in the chiral square cupola compound $BaTiOCu_4(PO_4)_4$

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We report neutron diffraction studies of the magnetic structure in BaTiOCu4(PO4)4 , which is a newly discovered magnetic insulator crystallizing in a tetragonal chiral crystal structure with P4212 space group [1]. The crystal structure is characterized by an antiferro-rotative arrangement of Cu4O12 square cupola clusters formed by four corner sharing CuO4 plaquettes. Below 9.5 K these magnetic clusters order in a complex noncollinear magnetic structure which can be described by an antiferroic order of magnetic quadrupole moments on Cu4O12 square cupolas.
The magnetic transition is accompanied by a magnetic-field-induced peak in dielectric constant divergent toward T = 9.5 K, indicative of an onset of field-induced antiferroelectric order [2]. To the best of our knowledge, this is the first experimental observation of the magnetoelectric-activity due to magnetic quadrupole moments [3], which opens the arena for further studies of this and related compounds.
In this presentation, we shall focus on the determination of the magnetic structure exploiting a combination of powder neutron diffraction and so-called spherical neutron polarimetry. The powder diffraction measurement was able to identify two possible models for the magnetic structure, as depicted in the figure. Both structures are noncollinear, but differ by having the moments either in or out of the CuO4 planes. Powder diffraction could only provide limited discrimination between the two models. Spherical neutron polarimetry is a convenient, albeit rarely used tool for understanding complex magnetic structures which often can provide unambiguous solutions to withstanding problems. In this case spherical neutron polarimetry unambiguously identifies structure (b) with the moments pointing out of the CuO4 planes.
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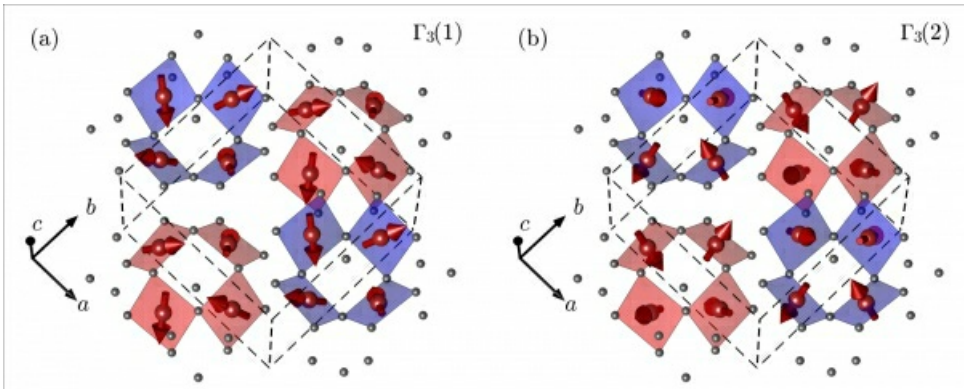

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