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Mechanism of the magnetically-induced ferroelectricity in $(\mathrm{ND}_4)_2$[$\mathrm{FeCl}_5 \cdot \mathrm{D}_2\mathrm{O}$] multiferroic molecular compound J. ALBERTO RODRIGUEZ-VELAMAZAN, Materials Science Institute of Aragon @ Institut Laue Langevin, OSCAR FABELO, Institut Laue Langevin, ANGEL MILLAN, JAVIER CAMPO, Materials Science Institute of Aragon, ROGER JOHNSON, Clarendon Laboratory Department of Physics University of Oxford, LAURENT CHAPON, Institut Laue Langevin — In magnetoelectric multiferroic materials, a subtle competition between different magnetic interactions is at the origin of multiferroicity, as this competition is the responsible of the formation of a magnetic structure able to induce ferroelectric polarization. The difficulty in controlling this interplay of interactions explains the scarce number of these materials reported. (ND4)2[FeCl5·D2O] is a rare case where improper ferroelectricity has been observed in a molecular material. We have used single crystal and powder neutron diffraction to study its crystal and magnetic structures and hence determine the mechanism of multiferroicity in this compound. From the crystal structure determinations above and below 79 K, we have observed an order-disorder phase transition, which is related with the ordering of the ammonium counterion. Below TN, at zero magnetic field, we have determined the magnetic structure, which corresponds with a cycloidal spin arrangement where the magnetic moments are contained in the ac-plane and propagate along the c-direction. All the cycloids in (ND4)2[FeCl5·D2O] compound have the same chirality and therefore the ferroelectricity can be explained via the inverse Dzyaloshinskii-Moriya mechanism.

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