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Understanding multiferroicity in the new $(ND4)_2$ FeCl₅ (D_2O) molecular magnet

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The family of antiferromagnetic A2[FeCl5(H2O)] compounds (A = alkali metal or ammonium ion) has awakened a renewed interest owing to the recent observation of multiferroicity in some of its members [1]. We have recently investigated by means of single crystal and powder neutron diffraction the magnetic structure of (ND4)2[FeCl5(D2O)] (with properties completely equivalent to the hydrogenated form) in order to understand the underlying mechanism of multiferroicity in this compound. This material orders antiferromagnetically at TN = 7.25 K and multiferroicity arises below ca. 6.9 K with the onset of ferroelectric order. We have observed at zero magnetic field a cycloidal magnetic structure propagating in the c-axis with k = (0, 0, 0.23) and with the magnetic moments lying in the ac plane (Fig 1). This cycloid would be at the origin of the magneto-electric coupling via inverse Dzyaloshinsky–Moriya interaction [2]. Also the evolution of the magnetic structure with increasing the magnetic field has been determined by the use of neutron diffraction under applied magnetic field. It shows three different regions including a lock-in of the propagation vector for fields between 2.5 and 5 T.

[1] Ackermann M, Brüning D, Lorenz T, Becker P and Bohatý L (2013) New J. Phys. 15 123001

[2] Rodríguez-Velamazán J.A., Fabelo O, Campo J, Millán A, Chapon L, Johnson R, Scientific Reports (2015) | 5:14475 | DOI: 10.1038/srep14475



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