Oral Contributions

[MS14-05] Crystal-Chemistry of new Low-D Ferromagnetic oxides: Influence of aperiodicity and cationic ordering on the magnetic properties

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Low-dimensional oxides with disconnected magnetic units are of increasing interest due the peculiar properties and the versatile interplay between individual magnetic moments into an external magnetic field. Our group is interested in the elaboration of such modular new compounds and their characterization by combining experimental (XRD, ND, magnetic) measurements and theoretical calculations [1]. Our main strategy focuses on 3-, 4- X_2O_7) magnetic sub-units formed of anisotropic magnetic ions (Fe^{2+}, Co^{2+}) isolated by big spacers (Ba^{2+}, PO4 Here, we present several new compounds in which the magnetic properties are mediated by complex structural features, including : -$BaFe_2(PO_4)_2$ was recently prepared in hydrothermal conditions and identified as the first 2D-Ising ferromagnetic (FM) oxide, Tc =65.5K. It contains isolated *honeycomb* layers made up of edge-sharing FeO6 octahedra with high-spin Fe^{2+} ions (S=2) [2] (Figure 1a). On cooling, $BaFe_2(PO_4)_2$ undergoes a rare re-entrant structural transition R-3(RT)→P-1(140 K)→R-3(Tc) due to *Jahn–Teller* distortion in competition with FM magnetostrictive effects [3]. Furthermore, around 700K, it undergoes a topotactic and reversible Fe ex-solution into several ordered superstructures containing new Fe-depleted triangular lattices with mixed valence Fe^{2+}/Fe^{3+}. The relationships between the crystal structures and the versatile magnetic properties will be discussed on the basis of accurate crystal structures refined by single-crystal XRD.

-Another striking example concerns the BaCo(X2O7) series (X=P, As). We will show how an incommensurate structural modulation assorted with strong atomic displacements is responsible for magnetization steps under an applied field. Briefly, the displacement waves transform the Co^{2+} 1D-chains topology (average structure, spacegroup P-1) into 2D-layers (4D-model; superspacegroup P-1(αβγ)0 ;q~0.13, 0.08, 0.48) (figure 1b) with a distribution of strongly Co^{2+} triangles **[4]**. The exchanges calculated by DFT (according with magnetic structu re determined by ND at 0T), show that they are mainly responsible for the stepped magnetization along AFM• FERRI• FM transitions.

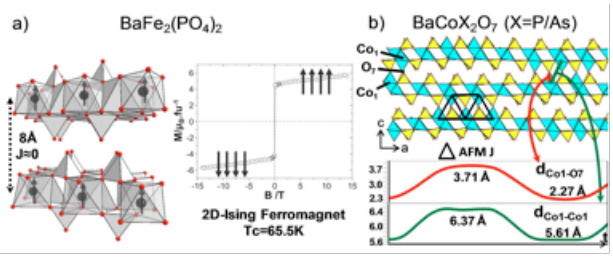

Figure 1 : *a) description of $BaFe_2(PO_4)_2$ structure and magnetic curve; b) description of the structural modulation in $BaCoX_2O_7$ and evidence of the frustration triangles.*

[1] R. David, A. Pautrat, H. Kabbour, M. Sturza, S. Curelea, G. André, D. Pelloquin *Chem. Mater.* **2011**, 23, 5191

[2] H. Kabbour, R. David, A. Pautrat, H-J. Koo, M-H. Whangbo, G. André, O. Mentré, *Ang. Chem.*, Int. Ed. **2012**, 51, 11745

[3]*«Across the structural re-entrant transition in $BaFe_2(PO_4)_2$:Influence of the two-dimensional ferromagnetism»* R. David, A. Pautrat, D. Filimonov, H. Kabbour, H. Vezin,M.H. Whangbo, G. André, O. Mentré, submitted at J.

[4]*«Stuctural modulation promoting magnetization steps in $BaCoP_2O_7$»*, R. David, H. Kabbour, A.Pautrat, S. Colis, O. Mentré, submitted at *J. Phys.Chem. C.*

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