Interplay between *3d-3d* and *3d-4f* interactions at the origin of the magnetic ordering in the Ba_2LnFeO_5 oxides

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Context : *The magnetic interaction between 4f and 3d cations in insulating oxides is a challenging question that remains largely unsolved nowadays*

Aim of this study : **Investigate magnetic transitions involving 3d and 4f ions « acting on an equal footing »**

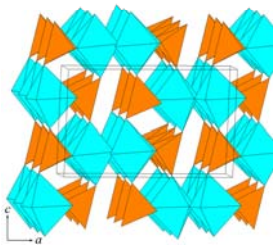
→ **Strategy ? : Cancel the 3d-3d SE ⇒ Balanced interplay between 3d-3d SSE and 3d-4f SE**

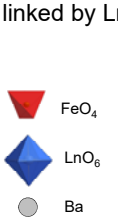
→ **Experimental realization ? : The $Ba2YFeO_5$-type structure** (K. Luo, M.A. Hayward, Inorg. Chem. 2012, 51, 12281)

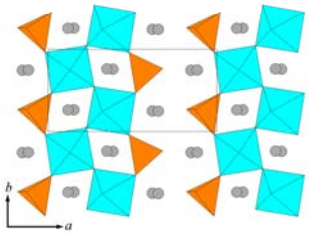
Abbreviations
SE=super-exchange
SSE=super-super-exchange
LRO=long-range ordering

Crystalline structure

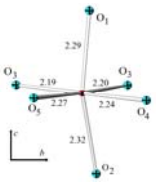
FeO_4 linked by LnO_6







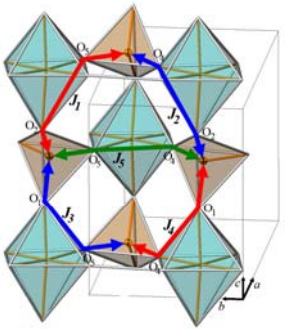
Distortion of the LnO_6



Ex. of Ba_2DyFeO_5

⇒ Single-ion anisotropy

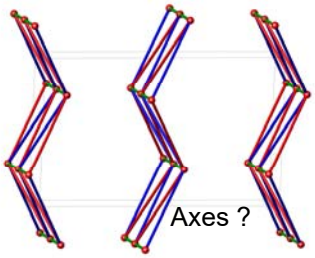
Magnetic interactions



No magnetic Ln

-5 main SSE 3d-3d couplings (SIMBO)

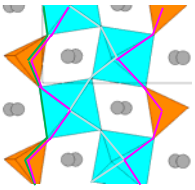
-2D character



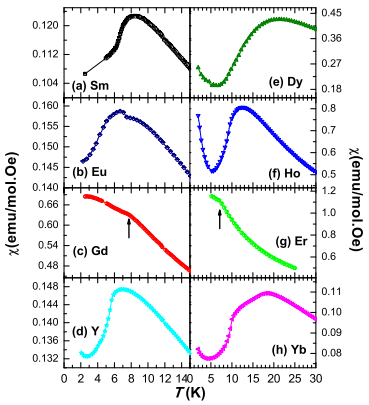
Adding magnetic Ln

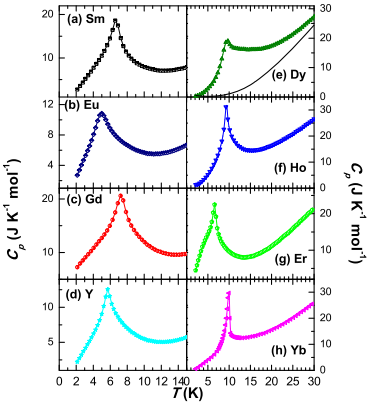
-SE 4f-3d

-SE 4f-4f (weaker)

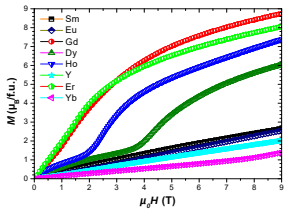


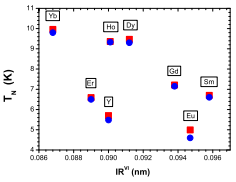
Long-range magnetic ordering





► Existence of a T_N in Ba_2YFeO_5
⇒ there is a LRO driven by 3d-3d SSE only
► No T_N in Ba_2DyGaO_5
⇒ no LRO (>2K) driven by 4f-4f SE only
► Unique T_N dependent on Ln in Ba_2LnFeO_5
⇒ rare example of LRO driven by an interplay between 3d-3d SSE and 3d-4f SE





Ln features impacting T_N ?
-not the ionic radius
-most likely the spin value
-probably the single-ion anisotropy

Magnetic structures

$$\Gamma_{Mag} = 3\Gamma_1^1 + 3\Gamma_2^1 + 3\Gamma_3^1 + 3\Gamma_4^1$$