MAGNETIC ANISOTROPY AND SPIN TRANSITION: WEIGHING THE FINE BALANCE OF LIGAND FIELD, SPIN ORBIT AND LATTICE EFFECTS.

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The magnetic anisotropy is a running paradigm of the nowadays molecular magnetism, stirring interest both from academic point of view, since it has intricate mechanisms, and also for application purposes, its understanding serving to design systems behaving as magnets at molecular and nano-scale levels. Placing on equal footing the experimental and theoretical deals, we had our own contribution of rationales in this quest,[1-4] offering new keys for this major keyword, by approaching several case studies and proposing useful new tools of analysis, such as the polar maps of state-specific magnetization functions. (Fig.1.A) In our recent works we presented strong advances in the magnetic anisotropy determined by the interplay of Ligand Field and Spin Orbit effects. These factors are also important in spin conversion phenomena, intervening also the factors of long range intermolecular interactions. Having as primary goal the magnetic anisotropy of compressed vs. elongated Mn(III) octahedral complexes, we serendipitously entered the field of spin conversion identifying systems with unusual spin behavior[5], performing a thorough analysis of structure-properties relationship. Molecular and supramolecular factors are discussed. Particularly, we rationalized the interplay of the vibrational factors into the electronic levels, simulating the details of the spin crossing mechanisms. (Fig.1.B)

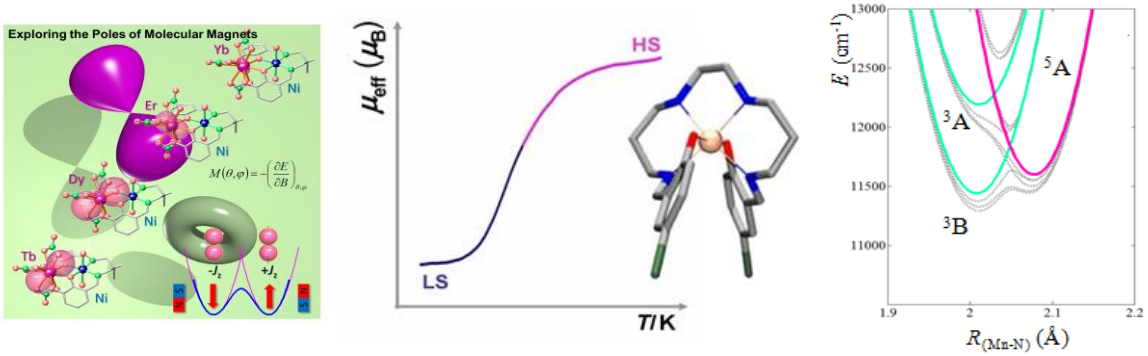


Figure 1. A. Simulated magnetization polar surfaces for a family of d-f SMMs with respect of molecular frame. **B.** The spin conversion effects of the Mn(III) complex with the N,N'-Bis(3-aminopropyl) ethylene diamine, 5-bromo-salicylaldehyde ligand: temperature driven magnetic moment variation. **C.** states involved in the spin transitions

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