Understanding the origin of magnetic anisotropy in S=1/2 mononuclear transition metal complexes

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Magnetic anisotropy is a key property along with the molecular spin in order to generate molecules that exhibit single molecule magnet behavior. For systems with total spin S=1/2, the presence or absence of magnetic anisotropy can be explained by means of the molecule's g-tensor. Using ideal models to screen the most common geometries for coordination numbers 2 to 8 in mononuclear transition metal complexes, we employed the Ab initio Ligand field Theory (AILFT)[1] formalism as implemented in the electronic structure package ORCA[2] to build a qualitative model to predict the behavior of the magnetic anisotropy in molecular systems with S = 1/2. This model has been validated against available experimental information in order to examine our predictions. We will also show the potential use of this model to design new molecules exhibiting large magnetic anisotropy.

1. (a) M. Atanasov, D. Ganyushin, K. Sivalingam and F. Neese, *Structure and Bonding*, ed. D.M.P. Mingos, P. Day and J.P. Dahl, Springer, Berlin, 149–220 (2012); (b) M. Atanasov, D. Aravena, E. Suturina, E. Bill, D. Maganas and F. Neese, *Coord. Chem. Rev.* **289** 177 (2015).
2. F. Neese, *Wiley interdisciplinary Reviews – Computational Molecular Science*. **2** 73-78 (2012).