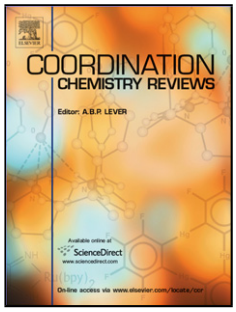

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Large Magnetic Anisotropy in Mononuclear Metal Complexes

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Contents

Abstract

This review examines mononuclear metal complexes with high magnetic anisotropy and the theoretical approaches used to rationalize their magnetic properties. Electronic structure calculations based on CASSCF (or CASPT2/NEVPT2) methods provide a quantitative agreement of the zero-field splitting parameters either for mononuclear transition metal complexes or for equivalent lanthanide systems. To produce a more qualitative tool for predicting the magnetic anisotropy of metal complexes, we have developed a set of simple models. For transition metal systems, a simple model based on the splitting of the *d* orbitals, considering the coordination mode of the metal and its electronic configuration, is enough to qualitatively predict the system's magnetic anisotropy. A similar approach does not work with the *f* orbitals of the lanthanide complexes. As an alternative, we studied the electrostatic field generated by the ligands and found that this magnitude controls the shape and the orientation of the anisotropic electron density. This procedure allows us to rationalize and to predict whether the system will have a strong axial character, and also to determine the direction of the magnetic moment.

Keywords: Magnetic Anisotropy, *ab initio* Calculations, Single-Molecule Magnets, Molecular Magnetism