Title: Study of the Magnetic Anisotropy of Mononuclear Intermediate Spin Complexes
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Intermediate spin systems are an unusual situation in Coordination Chemistry. A subtle energy balance between the usual high- and low- spin states leads to such electronic configuration. In this work, the magnetic anisotropy of different intermediate spin compounds has been analysed in order to check if they could present single-molecule magnet behaviour. First of all, a general search of compounds with similar geometry to that of reported intermediate spin compounds has been done using the Cambridge Structural Database. A qualitative model using the orbital energies of the d orbitals to predict the anisotropy depending on geometry and electronic configuration has been employed. Lastly, the available experimental data of the reported intermediate spin compounds have been compared and discussed with the predictions of our model.

Keywords: Intermediate spin, SMM (Single-Molecule Magnets), magnetic anisotropy, CSD (Cambridge Structural Database).