

Title: **Magnetic study of Single Molecule Magnets with spin 1/2**

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Single Molecule Magnets (SMMs) are molecules capable of retaining their magnetization in the absence of an external magnetic field, or in other words, they can behave as small magnets. During the last years, they have been proposed for data storage and as spin qubits in quantum computing. In the group where this work has been carried out, they have studied and modelled the magnetic properties of SMMs in the past years. Recently in the group, a model has been created to predict the magnetic properties of mononuclear complexes with spin $\frac{1}{2}$. In this work that model has been revised with different energy criteria. From the predictive model several coordination geometries will be proposed as candidates with interesting magnetic properties. A search in the Cambridge Structural Database will be performed and using the Shape program the best candidates will be selected. Those candidates will be proposed to be synthesized and for further study of their interesting magnetic properties.