

Single-ion anisotropy effects in magnetic susceptibility of some Re^{IV} and $\text{Re}^{\text{IV}}\text{M}^{\text{II}}$ complexes

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In this communication we analyse the effects of single-ion anisotropy on the zero-field susceptibility behaviour as a function of temperature for an oxalate- Re^{IV} mononuclear complex [1] and heterotetranuclear oxalato-bridged $\text{Re}^{\text{IV}}\text{M}^{\text{II}}$ ($\text{M} = \text{Mn}, \text{Fe}, \text{Ni}, \text{Cu}$) complexes [2]. Re^{IV} is a $5d^3$ ion which ground state in the octahedral environment is given by the $^4A_{2g}$ term and is subject to a high value of the spin-orbit coupling and the strong magnetic anisotropy. Our analysis is based on the spin Heisenberg model and takes into account both the uniaxial and rhombic single-ion anisotropy term. We calculate within the exact diagonalisation technique the single-crystal and powder susceptibility for the systems in question. We find some symmetries in the behaviour of the single-crystal susceptibilities and their substantial dependence on the value of the rhombic parameter. We demonstrate that the differences in the single-crystal data are strongly reduced for the powder sample and we estimate some new values of the model parameters from a fit to experimental data.

[1] R. Chiozzone et al., *Inorg. Chem.* 38, 4745 (1999)

[2] J. Martinez-Lillo et al., *Inorg. Chem.*, 48, 3027 (2009)

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