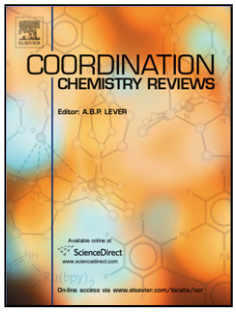

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PII: S0010-8545(14)00284-7
DOI: http://dx.doi.org/doi:10.1016/j.ccr.2014.10.011
Reference: CCR 111949

To appear in: *Coordination Chemistry Reviews*

Received date: 10-7-2014
Revised date: 27-10-2014
Accepted date: 30-10-2014

Please cite this article as: J. van Leusen, M. Speldrich, H. Schilder, P. Kögerler, Comprehensive insight into molecular magnetism via CONDON: full vs. effective models, *Coordination Chemistry Reviews* (2014), http://dx.doi.org/10.1016/j.ccr.2014.10.011

Comprehensive insight into molecular magnetism via CONDON: full vs. effective models

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Abstract

Analyzing the magnetic properties of molecular compounds means unraveling the electronic multiplet structure and properties of molecules on a small-energy scale. Various models have been introduced in the past to describe molecular magnetic characteristics, and to overcome associated limits of computational resources. Herein, model calculations based on effective theory, ligand-field theory and ab initio methods are critically compared and discussed. Using our computational framework CONDON, selected examples of magnetically anisotropic lanthanide and actinide systems point out their drawbacks and opportunities, and explicitly reveal exaggerated statements found in literature regarding their applicability and potentials.

Keywords: magnetic properties, molecular magnetism, molecular modeling, theoretical chemistry, lanthanide compounds, actinide compounds

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