

MAGNETISM AND MAGNETIC MATERIALS

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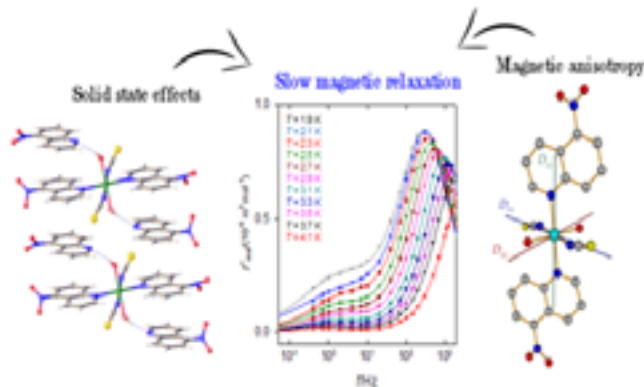
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INVESTIGATION OF MAGNETIC MOLECULES CONTAINING 3D AND 4F METALS

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Rationally designed magnetic molecules, such as single-molecule magnets (SMMs), are regarded as potential candidates for various applications in future molecular electronics. SMMs are above all transition metal and/or lanthanide complexes that, beside other interesting quantum phenomena, exhibit slow relaxation of the magnetization at the level of one molecule. We have studied a series of metal complexes containing Co(II), Ni(II) and Dy(III) ions showing multiple field-supported slow magnetic relaxation processes detected by AC susceptibility measurements. A set of AC magnetic parameters (isothermal susceptibilities, distribution parameters, relaxation times) have been fitted to the experimental data by employing the multiple (two, three)-set Debye model. Static (DC) magnetic properties of these compounds were also studied experimentally and theoretically. By employing the standard spin Hamiltonian, we have extracted the DC magnetic parameters (*g*-factor components, zero-field splitting parameters). By combining the structural and magnetic experimental data and quantum chemistry calculations (DFT, *ab initio*) we have defined the magnetostructural correlations which provide simple rules for tuning the SMM properties in this family of compounds.



Recent Publications

1. Lomjanský D, Moncol J, Rajnák C, Titiš J, Boča R (2017). Field effects to slow magnetic relaxation in a mononuclear Ni(II) complex. *Chemical Communications*. 53:6930-6932.
2. Boča R, Stolárová M, Falvello LR, Tomás M, Titiš J, Černák J (2017). Slow magnetic relaxations in a ladder-type Dy(III) complex and its dinuclear analogue. *Dalton Transactions*. 46:5344-5351.
3. Hazra S, Titiš J, Valigura D, Boča R, Mohanta S (2016). Bis-phenoxido and bis-acetato bridged heteronuclear {CoIIIDyIII} single molecule magnets with two slow relaxation branches. *Dalton Transactions*.

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4. Smolko L, Černák J, Dušek M, Titiš J, Boča R (2016). Tetracoordinate Co(II) complexes containing bathocuproine and single molecule magnetism. *New Journal of Chemistry*. 40:6593-6598.
5. Banik R, Roy S, Dlhán L, Titiš J, Boča R, Kirillov AM, Martin AD, Bauza A, Frontera A, Rodríguez-Diéguez A, Salas JM, Das S (2016). Self-assembly synthesis, structure, topology, and magnetic properties of a mononuclear Fe(III)-violurate derivative: A combined experimental and theoretical study. *Dalton Transactions*. 45:16166-16172.

BIOGRAPHY

Ján Titiš has completed his PhD in 2008 from Slovak University of Technology. He is the Associate Professor of Inorganic Chemistry at University of Ss. Cyril and Methodius in Trnava and Executive Coeditor of *Nova Biotechnologica et Chimica*. He has published 55 papers in reputed journals. His h-index is 12.

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