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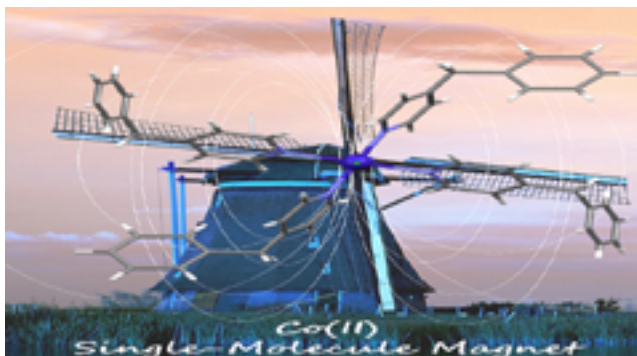
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## FIELD SUPPORTED SLOW MAGNETIC RELAXATION IN HEXACOORDINATE CO(II) COMPLEXES WITH EASY PLANE ANISOTROPY

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Single molecule magnets known up to date cover several classes of transition metal complexes: there are polynuclear and mononuclear, 3d and 4f, heteronuclear 3d-4f, field induced, and field suppressed, with single mode and multimode relaxation channel systems. Over the past years an increased interest is paid to mononuclear 3d complexes mainly for their easy synthesis, stability, and low price. They involve high-spin Cr (III), Mn (III), Fe (III), Fe (II), Fe (I), Co (II), Ni (I), and Ni (II) complexes. Also, the key factor – the magnetic anisotropy is much easily tuned by a rational synthesis for mononuclear complexes. Considerable attention has been paid to the class of mononuclear Co (II) complexes, mostly tetracoordinate, pentacoordinate, and hexacoordinate. These complexes possess a large magnetic anisotropy expressed by the axial zero-field-splitting (ZFS) parameter D. However, the language in terms of the D- and E-parameters implies that the spin Hamiltonian formalism is legitimate to apply which holds true only for the non-degenerate ground electronic terms of the A- or B-symmetry (point-group irreducible representation); this is the case of quasitetrahedral Co (II) complexes. For pentacoordinate and hexacoordinate complexes one should be careful since here also the degenerate ground electronic terms occur: 4E for the geometry of tetragonal pyramid (the coordination number  $cn=4+1$ ) and 4Eg for the elongated tetragonal bipyramid ( $cn=4+2$ ). Application of the spin Hamiltonian (SH) formalism to magnetic data fitting and/or ab initio calculations for systems with degenerate ground term is conceptually mistaken since SH approach utilizes the non-degenerate perturbation theory.



### Recent Publications

- Schäfer B, Rajnák C, Šalitroš I, Fuhr O, Klar D, Schmitz-Antoniak C, Weschke E, Wende H, Ruben M (2013). Room temperature switching

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of a neutral molecular iron(ii) complex. *Chemical Communications*. 49:10986-10988.

- Rajnák C, Titiš J, Fuhr O, Ruben M, Boča R (2014) Single-molecule magnetism in a pentacoordinate cobalt(II) complex supported by an antenna ligand. *Inorganic Chemistry*. 53:8200-8202.
- 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.
- Boca R, Rajnák C, Titis J, Valigura D, (2017) Field supported slow magnetic relaxation in a mononuclear Cu(II) complex. *Inorganic Chemistry*. 56:1478-1482.
- Rajnák C, Varga F, Titiš J, Moncol' J, Boča R (2017) Field-Supported Single-Molecule Magnets of Type [Co(bzimpy)X<sub>2</sub>]. *European Journal of Inorganic Chemistry* 2017:1915-1922.

## BIOGRAPHY

Cyril Rajnák has obtained an MSc and then a RNDr from the University of Ss. Cyril and Methodius in 2009 and 2010, respectively. He received his PhD from the University of Strasbourg in 2014 under the guidance of Prof. Mario Ruben. He received second PhD from the University of Ss. Cyril and Methodius under the supervision of Prof. Roman Boča. In 2015, he joined the Alma Mater as an Assistant Professor. His research is focused on organic and inorganic synthesis and development of single-molecule (Ion) magnets. He has published more than 20 reputed journals.

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