

NOVEL DESIGN OF MONONUCLEAR HEXACOORDINATED CO(II) COMPLEXES WITH SINGLE-ION MAGNET BEHAVIOR

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Novel design of mononuclear Co(II) coordination compounds with chemically stable coordination number six showing single-ion magnet properties is proposed. Rigid tetradentate ligand capable to form three chelate cycles (5+5+5) dictates heavily distorted (trapezoid) coordination environment in the plane of the ligand. With two additional monodentate ligands hexacoordination environment of metal center is formed with local axial C₂ symmetry. Two compounds I (A = Cl⁻, NCS⁻) of such type were synthesized and their magnetic susceptibility in DC and AC magnetic fields was studied [1]. Both compounds show large axial zero-field splitting (ZFS) and field-induced slow relaxation of magnetic susceptibility in AC field.

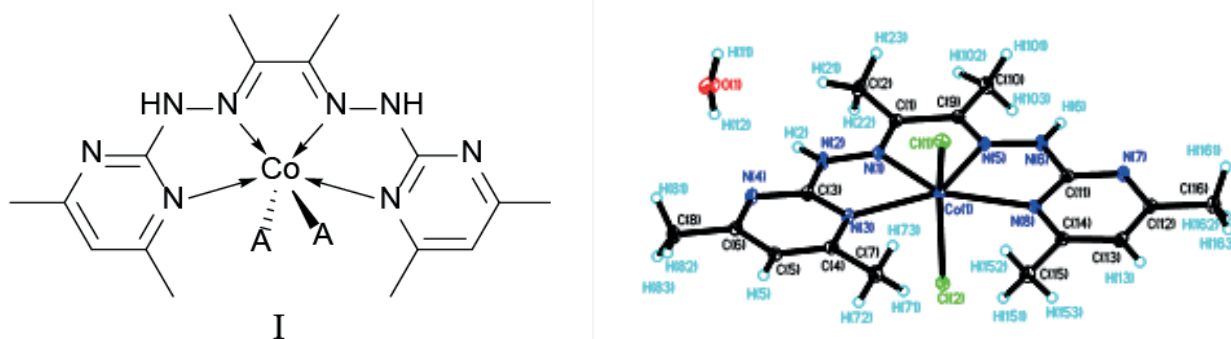


Fig.1. Complexes I (A=Cl⁻, NCS⁻), molecular structure of I, A = Cl⁻

Presence of solvation water molecules in crystal structure of I (A=Cl⁻, see Fig.1) results in formation of intermolecular hydrogen bond network favoring weak antiferromagnetic exchange interaction between paramagnetic centers. In I (A=NCS⁻) DMSO molecule is present, preventing exchange interaction between Co(II) ions. Quantum-chemical modelling of ZFS parameters were performed at CASSCF/NEVPT2 theory level.

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References

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