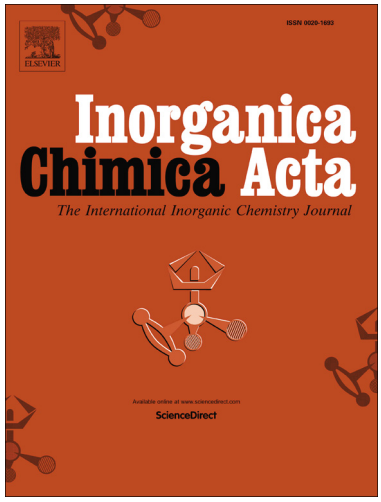

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Pentacoordinate cobalt(II) complexes with neutral tripodal *N*-donor ligands: zero-field splitting for a distorted trigonal bipyramidal geometry

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Abstract

A series of pentacoordinate Co(II) complexes of the composition [Co(bpdmpz)Cl]ClO_4 (**1**), [Co(bpdmpz)Cl]PF_6 (**2**), [Co(bdmpzp)Cl]$ClO_4 \cdot H_2O$ (**3**), [Co(bdmpzp)Cl]PF_6 (**4**), [Co(tdmpza)Cl]ClO_4 **(5)** and [Co(tdmpza)Cl]PF_6 **(6)** (bpdmpz = bis[(2-pyridylmethyl)-(di(3,5-dimethyl-1H-pyrazolyl)methyl)]amine, bdmpzp = bis[(di(3,5-dimethyl-1H-pyrazolyl)methyl))-(2-pyridylmethyl)]amine and tdmpza = tris[di(3,5-dimethyl-1H-pyrazolyl)methyl)]amine) was prepared and thoroughly characterized. Single-crystal X-ray analyses of complexes **1**–**5** revealed that they possess very close molecular structures with a distorted trigonal bipyramidal geometry. The static DC magnetic experiments revealed the ZFS parameters pointing out small magnetic anisotropy (with the $|D|$ values lying in a relative narrow range of 4.4 – 5.7 cm^{-1}) and rhombicity (with the E/D parameters in the range of 0 – 0.26). The dynamic magnetic data revealed that AC susceptibility is temperature and frequency-dependent for **1**, **2** and **3**, and thus, these compounds belong to a group of field-induced pentacoordinate Co(II) single-molecule magnets (SMMs). The evaluation of magnetic data was also supported by the CASSCF/NEVPT2 calculations.

Keywords: Cobalt(II) complexes • Tripodal ligands • Crystal structure • Magnetic properties • Single-molecule magnets

1. Introduction

The molecular magnetism of transition metals, especially of Co(II), has revealed great progress since discovery of the first Co(II) mononuclear pentacoordinate compounds involving bis(imino)pyridine pincer ligands and exhibiting slow relaxation of magnetization (SRM) by Jurca et al.[1] The coordination compounds exhibiting SRM due to the existence of the spin reversal barrier (U) are called Single-Molecule Magnets (SMMs),[2] and such compounds are intensively studied materials for their possible