MS30-P34 Co(II) complexes with abpt ligands and pseudohalide anions exhibiting single-ion magnet behavior

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The early examples of nanomagnets exhibiting slow relaxation of the magnetization (single-molecule magnets (SMMs)) were clusters of transition metal ions but recently mononuclear complexes (called single-ion magnets, SIMs) have been reported [1], even with the positive axial parameter of zero-field splitting (D) [2]. Nevertheless, the origin of SIM properties in mononuclear Co(II) complexes with D>0 remains rather unclear and more examples of this type of compounds are needed to shed light on the subject. With these ideas in mind, we have prepared five centrosymmetric pseudooctahedral mononuclear Co(II) complexes with 4-amino-3,5-bis(2-pyridyl)-1,2,4-triazole (abpt) ligand and nonlinear pseudohalide anions: tricyanomethanide (tcm), nitrocyanamide (nca), nitrodicyanomethanide (nodcm), tetracyanoazapropenide (tcap), and pentacyanopropenide (pcp).

Equatorial plane in the $[Co(abpt)_2(tcm)_2]$ complex (**1**) is occupied by pairs of N2 and N3 atoms of two abpt and tcm ligands (Co1–N2 = 2.125(2) and Co1–N3 = 2.133(2) Å), pair of N1 atoms occupy axial positions at 2.109(2) Å (Fig. 1). This slightly compressed octahedral complex shows field-induced slow relaxation of magnetization with large axial single-ion zero-field-splitting parameter D = +48(2) cm^{-1} [3]. Similar structure exhibits $[Co(abpt)_2(nca)_2]$ (**2**) complex, with N2 and N3 atoms coordinated at 2.144(2) and 2.121(2) Å, respectively and N1 atoms coordinated at 2.086(2) Å. On the other hands, $[Co(abpt)_2(H_2O)_2]X_2$ (X = nodcm (**3**) and tcap (**4**)) and $[Co(abpt)_2(MeOH)_2](pcp)_2$ (**5**) complexes exhibit slightly elongated octahedral structures with equatorial planes occupied by pairs of N2 atoms of abpt and O3 atoms of water/methanol ligands at 2.112(2) and 2.118(2) Å (**3**), 2.081(1) and 2.102(1) Å (**4**), and 2.058(1) and 2.109(1) Å (**5**), respectively. N1 atoms occupy axial positions at 2.146(2) (**3**), 2.166(1) (**4**) and 2.151(1) Å. Nodcm (**3**), tcap (**4**) and pcp (**5**) anions remain uncoordinated.

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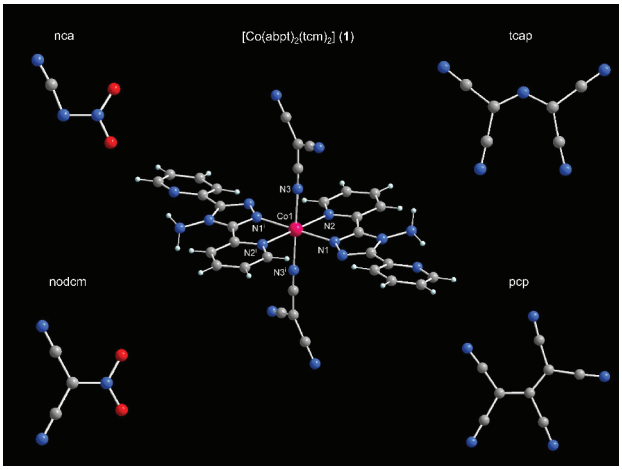

Figure 1. Structure of $[Co(abpt)_2(tcm)_2]$ complex (1) along with structures of nitrocyanamide (nca), nitrodicyanomethanide (nodcm), tetracyanoazapropenide (tcap), and pentacyanopropenide (pcp) anions used in complexes 2 – 5, respectively.

Keywords: Co(II) complexes, abpt, pseudohalides, single-ion magnets