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Structures of new Cu(II) and Co(II) 4-amino-1,2,4-triazole coordination compounds

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The coordination chemistry of NH_2trz (4-amino-1,2,4-triazole) has rapidly expanded due to the ability of this ligand to propagate elastic and magnetic interactions between transition metal ions, which are of great appeal in molecular magnetism. New coordination compounds with NH_2trz and dicyanamide (dca) bridging ligands, $[Cu(NH_2trz)_4(H_2O)](AsF_6)_2$ **1**, $[Cu(NH_2trz)_3](ZrF_6)\cdot H_2O$ **2**, and $[Co_3(NH_2trz)_8(dca)_4](dca)_2\cdot 2H_2O$ **3**, have been prepared and structurally characterized. In the mononuclear complex **1**, NH_2trz is monodentate and is coordinated through a nitrogen atom of the triazole ring with bond lengths Cu-N = 1.997(6) - 2.004(6) Å. Complex **1** has a square-pyramidal geometry. The coordination sphere is supplemented by a water molecule in apical position, at 2.276(9) Å from Cu(II). The metal centers in **2** are connected by three bidentate *N1,N2*-1,2,4-triazole ligands. It is an infinite 1D chain with Cu•••Cu = 3.8850(3) Å. The second coordination sphere is occupied by one non-coordinated water molecule and a hexafluoro-zirconate anion, which is situated between the linear chains. The interchain distance is 10.997(4) Å. The chains are connected by hydrogen bonds. There are two intermolecular interactions between fluorine and the non coordinated water molecule of the 1D chain. In **3**, the octahedral surrounding around one of the two Co ions is formed by three bidentate *N1,N2*-1,2,4-triazole ligands, with distances 2.130(4) - 2.142(4) Å. The cobalt ions located in the extremity of this trinuclear unit have an octahedral environment with two μ_1-dca molecules and monodentate NH_2trz coordinated through a nitrogen atom of the ring. The temperature dependence of the magnetic susceptibility of the linear trimer **3** indicates the presence of antiferromagnetic interactions between the cobalt ions.

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First nitrate complexes with chain structure.

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Nitrate complexes $Na_2[Co(NO_3)_4]$ (**I**), $K_2[Co(NO_3)_4]$ (**II**), $Ag[Co(NO_3)_3]$ (**III**) and $K_2[Ni(NO_3)_4]$ (**IV**) were prepared by crystallization from nitric acid solutions in the presence of P_2O_5 and were investigated by X-ray single crystal analysis. All these compounds crystallized in monoclinic crystal system (space group $P2_1/n$ for **I**, **II**, **III** and *Cc* for **IV**) with following parameters: a =0.759(1), b = 7.744(1), c = 11.801(1) Å, β = 92.923(9) °, V = 982.08(18) Å^3, R = 4.7 % (**I**); a = 6.826(1), b = 10.244(2), c = 15.088(3) Å, ß = 95.87(3) °, V = 1049.5(4) Å^3, R = 5.5 % (**II**); a = 7.576(5), b = 7.312(2), c = 12.838(5) Å, β = 94.18(4) °, V = 709.3(6) Å^3, R = 2.3 % (**III**); a = 16.739(3), b = 7.020(1), c = 9.050(2) Å, β = 98.67(3) °, V = 1051.3(4) Å^3, R = 1.8 % (**IV**). Structures **I** and **II** are island and are build from isolated anions $[Co(NO_3)_4]^{2-}$ and cations Na^+ and K^+ accordingly. All nitrate groups in complex anions $[Co(NO_3)_4]^{2-}$ of structure **I** are asymmetrical bidentate and coordination number (CN) of cobalt atom is 8. In the same time in anions $[Co(NO_3)_4]^{2-}$ of structure **II** one of four nitrate groups is monodentate and CN(Co) = 7. Compounds **III** and **IV** are the first nitrate complexes with chain structure. In anions $[Co(NO_3)_3]_n^{n-}$ of structure **III** cobalt atom is coordinated by seven oxygen atoms from one monodentate and three bidentate nitrate groups (Fig. 1a). Bridging nitrate group is bidentate to one cobalt atom and monodentate to neighbouring one. In structure **IV** in chains $[Ni(NO_3)_4]_n^{2n-}$ nickel atom is coordinated by five nitrate groups one of which is bidentate and two of monodentate nitrate groups are bridging (Fig. 1b). Comparison of stability of nitratocobaltates anions with different geometry was carried out by calculation of corresponding particles using program complex GAMESS.

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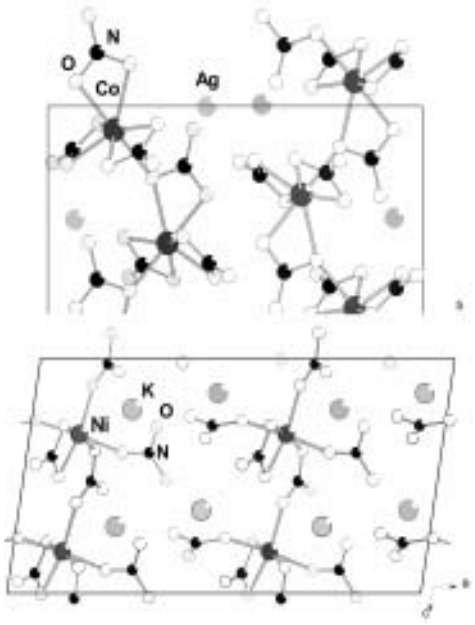

Fig. 1. Projection of the structure **III** onto plane *0bc* (a) and **IV** (b) onto plane *a0c* (b).