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LETTERS TO THE EDITOR

Synthesis and Crystal Structure of Mononuclear Nickel(II) Trifloroacetate Complex

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Currently, nickel(II) carboxylates are widely used as the starting materials for the synthesis of more complex systems [1, 2]. Typically, the synthesis of nickel carboxylates is carried out starting from the nickel hydrated oxide or carbonate and the corresponding carboxylic acid, as well as from the nickel(II) halide and the carboxylic acid salt. Note that these reactions afford fundamentally different complexes, depending on the properties of the substituent R of the carboxylate ligands. Thus, according to [3], reaction of the basic nickel carbonate with pivalic acid (PivH) at heating followed by crystallization from benzene gives a binuclear complex. The binuclear aqua-bridge complex $[Ni_2(\mu\text{-}OH_2)(\mu_2\text{-Piv-O,O'})_2(Piv)_2(PivH)_4]$ was obtained by heating (160°C, 3 h) of basic nickel(II) carbonate tetrahydrate with an excess of pivalic acid or by the boiling of nickel(II) hydroxide with PivH in toluene [4, 5]. The reaction of propionic acid with nickel(II) oxide in an autoclave (75°C, 48 h) results in a mixture of a polymer compound containing a binuclear lantern fragments $Ni_2(\mu\text{-}O_2CEt)_4$: $[Ni_2(\mu\text{-}O_2CEt)_4]_\infty$ and monomeric complex $[Ni_2(\mu\text{-}O_2CEt)_4(OH_2)_2]$ [6].

In this report the synthesis and the results of X-ray diffraction (XRD) study of the new mononuclear nickel(II) trifluoroacetate complex $[Ni(H_2O)_4(CF_3COO)_2]$ are described. The complex crystallizes in the monoclinic system with the space group *C*2/*c*, cell parameters: *a* 13.1135(10), *b* 12.7393(9), *c* 8.2399(6) Å, β 119.9770(10)°, *V* 1192.39 Å^3, *Z* 4, *Z*' 0, *R* 2.87%. This crystal structure formation is caused the hydrogen bonding between the carboxylate and aqua-ligands of the neighboring complex subunits.

In the complex the nickel atoms are located in the center of a tetragonal bipyramid, in whose terminal plane there are the coordinated water molecules. Two monodentate trifluoroacetate ligands coordinated by oxygen are located symmetrically above and below this plane. The IR spectroscopy data indicate a relatively low ionicity of Ni–O(O_2CCF_3) bond [7].

Nickel(II) (tetraaqua)bis(*O*-trifluoroacetate) (I). A fluoroplastic beaker (30 cm^3) charged with nickel(II) oxide (3 g, 0.04 mol) and trifluoroacetic acid (10 ml, 0.08 mol) was placed in a high pressure reactor. The reaction was carried out at 150°C for 1 day. After cooling, the reaction mixture is a solid crystalline phase and a small amount of turquoise-green liquid. The turquoise-green large prismatic crystals precipitate from the mother liquor after a few days. Yield 80% (relative to Ni). The complex is soluble in alcohol, acetonitrile, and water. Found Ni, %: 16.4. $C_4H_8F_6NiO_8$. Calculated Ni, %: 16.45. IR spectrum (KBr), ν, cm^{-1}: 3496.5 br [$\delta(H_2O)$], 1675.7 v. s [$\nu_{as}(COO)$], 1445.7 s [$\nu_s(COO)$], 1196.6 v. s and 1146.7 s (stretching vibrations, C–C), 861.9 w (out-of-plane bending vibrations of the O–H-dimer), 796.3 s, 730.8 s, 609.9 w, 521.0 w (overtone of C=O group).

Crystal data for the complex **I** are deposited in the Cambridge Structural Database (CCDC 803 963).

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