Crystal Structure and Synthesis of new Trinuclear 3d-metal Trifluoroacetates

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Anhydrous acid trinuclear trifluoroacetates of divalent metals $[M_3(CF_3COO)_6(CF_3COOH)_6]CF_3COOH$ where M = Ni (I) and Co (II), and partially hydrated nickel trifluoroacetate $[Ni_3(CF_3COO)_4(CF_3COOH)_4(H_2O)_4](CF_3COOH)_2$ (III) were synthesized and studied by X-ray diffraction. Compounds I and II were obtained by crystallization from solutions of $Ni(CF_3COO)_2 \cdot 4H_2O$ (I), $Co(CF_3COO)_2 \cdot 4H_2O$ (II) in trifluoroacetic anhydride in the presence of phosphoric anhydride as the drying agent. Compound I crystallizes in trigonal system, space group. R $\bar{3}$, Z=27, a = 13.307(2), c= 53.13(1) Å, V= 8148(2) $Å^3$, R_1 = 0.1112. The structure is molecular; trinuclear linear unit is formed by three metal atoms linked by trifluoroacetic bridges. Side atoms are connected with three trifluoroacetic acid molecules. Compound II crystallizes in triclinic system, space group P $\bar{1}$, Z=2, a = 13.199(6), b = 14.649(6), c = 15.818(6) Å, α= 90.04(4), β= 114.32(4), γ= 108.55(4)°, V= 2611.3(19) $Å^3$, R_1 =0.0480. Its structure resembles I, but it's more distorted. Compound III was obtained by crystallization from solution of $Ni(CF_3COO)_2 \cdot 4H_2O$ in trifluoroacetic acid (99%) in the presence of phosphoric anhydride as the drying agent. According to X-ray diffraction the data it crystallizes in triclinic system space group P $\bar{1}$, Z=1, a=9.121(18), b=10.379(2), c=12.109(2) Å, α=84.59(3), β=72.20(3), γ=82.80(3)°, V=1080.9(4) $Å^3$, R=0.0334. Unlike the previous compounds, here the metal atoms are linked by two trifluoroacetic groups and one water molecule.

Keywords: nickel trifluoroacetate, cobalt trifluoroacetate, crystal structure