



New coordination modes in potassium edta salts: $K_2[H_2\text{edta}] \cdot 2H_2O$, $K_3[H\text{edta}] \cdot 2H_2O$ and $K_4[\text{edta}] \cdot 3.92H_2O$.

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Streszczenie

Three potassium edta (edta is ethylenediaminetetraacetic acid, $H(4)Y$) salts which have different degrees of ionization of the edta anion, namely dipotassium 2-({2-[bis(carboxylatomethyl)azaniumyl]ethyl} (carboxylatomethyl)azaniumyl)acetate dihydrate, $2K^{+} \cdot C(10)H(14)N(2)O(8)(2^{-}) \cdot 2H(2)O$, (I), tripotassium 2,2'-({2-[bis(carboxylatomethyl)amino]ethyl}ammonio)diacetate dihydrate, $3K^{+} \cdot C(10)H(13)N(2)O(8)(3^{-}) \cdot 2H(2)O$, (II), and tetrapotassium 2,2',2'',2'''-(ethane-1,2-diylidinitrilo)tetraacetate 3.92-hydrate, $4K^{+} \cdot C(10)H(12)N(2)O(8)(4^{-}) \cdot 3.92H(2)O$, (III), were obtained in crystalline form from water solutions after mixing edta with potassium hydroxide in different molar ratios. In (II), a new mode of coordination of the edta anion to the metal is observed. The $HY(3^{-})$ anion contains one deprotonated N atom coordinated to K^{+} and the second N atom is involved in intramolecular bifurcated $N-H \cdots O$ and $N-H \cdots N$ hydrogen bonds. The overall conformation of the $HY(3^{-})$ anions is very similar to that of the $Y(4^{-})$ anions in (III), although a slightly different spatial arrangement of the $-CH(2)COO(-)$ groups in relation to (III) is observed, whereas the $H(2)Y(2^{-})$ anions in (I) adopt a distinctly different geometry. The preferred synclinal conformation of the $-NCH(2)CH(2)N-$ moiety was found for all edta anions. In all three crystals, the anions and water molecules are arranged in three-dimensional networks linked via $O-H \cdots O$ and $C-H \cdots O$ [and $N-H \cdots O$ in (I) and (II)] hydrogen bonds. $K \cdots O$ interactions also contribute to the three-dimensional polymeric architecture of the salts.

Adres publiczny

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