

Supramolecular motifs in the first structures of organic carboxylate salts of 1-(diaminomethylene)thiourea (HATU).

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Streszczenie

The structures of the first two organic carboxylate salts of 1-(diaminomethylene)thiourea (HATU), namely 1-(diaminomethylene)thiuron-1-ium formate, $C_2H_7N_4S^+.HCOO^-$, (I), and bis[1-(diaminomethylene)thiuron-1-ium] oxalate dihydrate, $2C_2H_7N_4S^+.C_2O(4)(2^-).2H_2O$, (II), in which the oxalate lies on a symmetry centre, possess different extended hydrogen-bonding networks with different graph-set motifs. The $R(2)(2)(8)$ motif present in (I) does not appear in (II), but an $R(2)(1)(6)$ motif is present in both (I) and (II). Compound (I) has a three-dimensional hydrogen-bonding network, whereas (II) has a layered structure with layers joined by hydrogen-bonding motifs that form $R(4)(2)(8)$ patterns. This work extends the known supramolecular structural data for HATU to include these organic carboxylates in addition to the previously characterized salts with inorganic acids.

Adres publiczny

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