

A New Supramolecular Assembly Obtained by Reaction Between Thiosaccharin and Hexamethylenediamine

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The crystal structure of hexamethylenediammonium bis(thiosaccharinate) dihydrate, $[\text{H}_3\text{N}-(\text{CH}_2)_6-\text{NH}_3](\text{tsac})_2 \cdot 2 \text{H}_2\text{O}$ (tsac = $\text{C}_7\text{H}_4\text{NO}_2\text{S}_2$, the anion of thiosaccharin), was determined by single-crystal X-ray diffraction. It crystallizes in the monoclinic space group $P2_1/a$ with $Z = 4$. The thiosaccharinate moiety is planar and shows small but significant modifications in the bonding of the thioamide functional group as compared with the protonated neutral molecule. The ionic crystal is further stabilized by an extensive H-bonding network, which links the anions and cations into an infinite three-dimensional supramolecular assembly. The FTIR spectrum of the compound is briefly discussed in comparison with those of the neutral constituent molecules.

Key words: Hexamethylenediammonium Bis(thiosaccharinate) Dihydrate, Crystallographic Data, Supramolecular Adduct, IR Spectra