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Hydrogen Bonding of O-Ethylxanthate Compounds and Neutron Structural Determination of C–H • • • S Interactions

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The hydrogen bonding in mixed sulfur/oxygen acceptor systems can be thoroughly investigated using the O-ethylxanthate (or O-alkyldithiocarbonate) family of anions. A series of O-ethylxanthate salts (guanidinium, methylammonium, dimethylammonium, trimethylammonium, tetramethylammonium, tetraethylammonium, and tetrapropylammonium), were structurally characterised using synchrotron X-ray spectroscopy to demonstrate the influence of the cation on the overall packing of the salts into either 3-D, 2-D or 1-D hydrogen-bonded arrangements. The protic cations vary in the number of available hydrogen bond donors which in turn affects the dimensionality of the hydrogen-bonded networks that form. The guanidinium cation gives rise to a 3-D hydrogen-bonded network due to the large number of NH hydrogen bond donors, whereas the use of ammonium cations, of the nature $\text{Me}_x\text{H}_4\text{--xN}^+$ ($x = 1\text{--}3$), demonstrates the decreasing dimensionality of the structures as the number of hydrogen bond donors decreases. Aprotic cations were also studied to demonstrate the influence of C–H...S interactions on the overall packing arrangement of the structure, in the absence of strong hydrogen bond donor groups. Laue neutron diffraction data was used to locate weak C–H...S hydrogen bonds in $(\text{Me}_4\text{N})(\text{EtXn})$ through the location of the exact positions of the CH hydrogen donors. The neutron data demonstrates the unequivocal presence of CH • • • S hydrogen bonding, with the H • • • S distance significantly shorter than the sum of the van der Waals' radii (shortest interaction 2.67 Å compared with 3.00 Å).

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