ABSTRACT

The Room Temperature Molecular and Lattice Structures and Thermotropic Phase Transition Behaviour of a Homologous Series of Anhydrous Zinc(II) \(n\)-Alkanoates

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The room temperature structures of a homologous series of zinc(II) \(n\)-alkanoates from chain length, \(n_c = 4 - 20\), inclusive, have been proposed using infrared (IR) spectroscopy, X-ray diffraction and polarizing light microscopy as well as density data and molecular model calculations. The data indicate that the compounds are isostructural, in that, each tetrahedral zinc ion is unsymmetrically coordinated to oxygen atoms from four different alkanoate groups and each ligand forms a Z,E-type bidentate bridge with two zinc ions resulting in a syn-anti arrangement. The hydrocarbon chains are in the fully extended all-trans conformation and are tilted at an average angle of 60 ° to the zinc basal planes and arranged in a tail-to-tail double bilayer for the shorter chain length homologues, \(n_c = 4 - 8\) and a head-to-tail double interdigitated bilayer for the longer chain lengths homologues, \(n_c = 9 - 20\). Geometric models are presented to account for odd – even chain effects in melting points and densities between these adducts. Overall, the lattice structures can be described as a three-dimensional polymeric, sheet-like, layered network.
Keywords: Zinc(II) n-alkanoates, X-ray single crystal and powder diffraction, Differential scanning calorimetry, Infrared spectroscopy, Polarizing light microscopy, Lamellar bilayer, Interdigitating bilayer, Z,E-type bidentate bridge, Polymeric layered network, Thermotropic phase behaviour, Intermediate transitions, Odd – even behaviour.