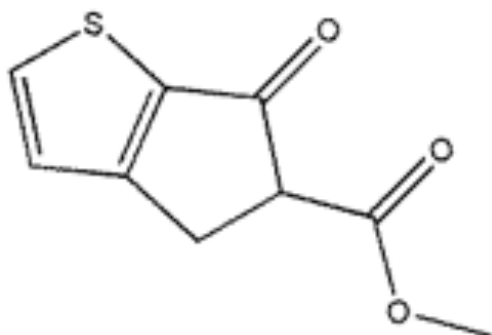


Poster Presentations

[MS10-P02] **Size does matter. Alkali metal complexes of a thiophene carboxy-enolate ligand.** Jim Simpson, Lyall R. Hanton, C. John McAdam and Stephen C. Moratti

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Our interest in conducting thiophene polymers and their incorporation into molecular actuators [1,2] led us to examine the potential use of methyl 6-oxo-5,6-dihydro-4H-cyclopenta[b]thiophene-5-carboxylate (I), shown below, as a ligand to a series of alkali metals. Examination of the Cambridge Structural Database [3] reveals only six structures incorporating the cyclopenta[b]thiophen-6-one skeleton with no reports of them having been used as ligands to generate coordination compounds.



(I)

We have prepared and structurally characterised complexes of the Li^+ , Na^+ and K^+ cations with (I) as a ligand and find that the structures of the resulting complexes are crucially dependent on the size of the metal. The Li^+ derivative, which crystallises as a monohydrate, is a simple, approximately tetrahedral, four co-ordinate complex with the metal chelated by the two $\text{C}=\text{O}$ oxygen atoms of the thiophenone ligand and carrying two additional water molecules. In the crystal a complex network of classical and non-classical hydrogen bonds stack the molecules along the *b* axis. The sodium complex is a dimer

that lies about an inversion centre. Each Na^+ cation is in a distorted trigonal bipyramidal coordination environment with the two cations bridged by two water molecules. The thiophenone ligand in this instance is monodentate through the carbonyl O atom of the carboxylate with the coordination sphere completed by two terminal aqua ligands. Packing of the sodium dimers is governed by an eclectic mix of $\text{O}\cdots\text{H}\cdots\text{O}$ and $\text{C}\cdots\text{H}\cdots\text{O}$ hydrogen bonds and short $\text{O}\cdots\text{S}$ contacts that stack the dimers along the *b* axis. The potassium cations form a three dimensional coordination polymer with each metal seven co-ordinated by one bridging and one terminal water molecule and three thiophenone ligands, two as bidentate chelates through the two $\text{C}=\text{O}$ oxygen atoms and the third monodentate through the thiophene S atom. The overall coordination geometry about each K^+ cation is approximately capped trigonal prismatic. The polymer forms infinite columnar stacks along the *c* axis with adjacent stacks linked by $\text{C}\cdots\text{H}\cdots\text{O}$ hydrogen bonds.

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