

**[o.m12.p11] The Crystal Structure of *n*-Octadecylammonium Bromide.** D.G. Billing, G.J. Kruger, M. Rademeyer, *Department of Chemistry and Biochemistry, Rand Afrikaans University, Johannesburg, 2006 South Africa.*

Keywords: surfactants, emulsifiers, bactericides.

Within our laboratory, we are currently investigating the crystal chemistry of a range of aliphatic materials. Including among these are the *n*-alkyl ammonium halides, which find applications as surfactants, emulsifiers, lubricants, bactericides and detergents. A number of investigations into the structures of *n*-alkyl ammonium chlorides have already been undertaken. We were interested in effect the introduction of a more bulky anion, would have on the packing of the alkyl chain.

The title compound was prepared by dissolving *n*-octadecylamine in chloroform, adding the acid halide and subsequently filtering off the *n*-alkylammonium halide product. Crystals suitable for single crystals studies were obtained by slow evaporation from hexane.

The structure solved readily within the spacegroup  $C_2$ , and refined to a final  $R$  of \_\_\_\_\_. Closer inspection of the structure however revealed the existence of a number of questionably long C—C bonds. Reminiscent of those reported by Nyburg for the di-*n*-octadecylammonium bromide crystal structure<sup>1</sup>.

In an attempt to address these shortcomings in the structure we repeated the structure analysis, using data obtained from another crystal on a SMART diffractometer. As no meaningful improvement resulted, we subsequently repeated the study at low-temperature, as well as performing a Rietveld refinement using powder diffraction data.

Here we would like to present, and critically compare the results we obtained for the various structural techniques used.

**[o.m12.p12] Structural and spectroscopic characterisation of complexes of mercury(II) halides and pseudo-halides with benzimidazole-2-thione.** D. Matkovic-Calogovic<sup>a</sup>, G. Pavlovic<sup>a</sup>, Z. Popovic<sup>a</sup>, Ž. Soldin<sup>a</sup> and G. Giester<sup>b</sup>, <sup>a</sup>*Laboratory of General and Inorganic Chemistry, Faculty of Science, Chemistry Department, University of Zagreb, Ul. kralja Zvonimira 8, HR-10000 Zagreb, Croatia,* <sup>b</sup>*Institut für Mineralogie und Kristallographie, Geozentrum, Universität Wien, Althanstraße 14, A-1090 Wien, Austria*

Keywords: mercury(II) complex, benzimidazole-2-thione, structure.

Our current interest in the coordination chemistry of mercury(II) complexes containing ligands with sulphur atoms is related to mercury-cysteine thionato interactions in various proteins. Soft ions such as mercury(II) tend to form complexes with S-donating ligands rather than N- or O- donating ones.<sup>1,2,3</sup>

A series of complexes  $HgX_2(bzimtH_2)$ ,  $HgX_2(bzimtH_2)_2$  ( $X = Cl, Br, I, SCN$ ;  $bzimtH_2 =$  benzimidazole-2-thione) has been obtained by the reaction of mercury(II) salts and benzimidazole-2-thione in the 1:1 and 1:2 molar ratio. Mercury(II) acetate yields  $Hg(bzimtH)_2$ . Complexes were characterised by IR spectra, <sup>1</sup>H and <sup>13</sup>C NMR measurements. The greatest complexation effects on chemical shifts in NMR spectra were detected for C-2 and H-1,3 atoms.

The crystal structure analysis of  $Hg(SCN)_2(bzimtH_2) \cdot C_2H_5OH$  (**1**),  $HgI_2(bzimtH_2)_2$  (**2**) and  $HgI_2(bzimtH_2)$  (**3**) revealed S-bound  $bzimtH_2$ . In the crystal structure of the 1:2 complexes there are isolated molecules with tetrahedrally coordinated Hg (two  $bzimtH_2$  ligands and two X ligands). The Hg-S( $bzimtH_2$ ) distance weakens with decreasing electronegativity of X [Hg-S 2.49(1) and 2.53(1) Å in **1** and 2.612(2) and 2.639(3) Å in **2**]. Structure **3** is polymeric as is often the case in the crystal structures of the 1:1 type of complexes. The characteristic coordination of mercury is trigonal with one  $bzimtH_2$  ligand and two I atoms at distances close to the sum of covalent radii of trigonal Hg and S or I [Hg-S 2.462(3) Å]. Additional weak Hg...I contacts at distances less than the sum of the van der Waals radii increase the effective coordination sphere to trigonal bipyramidal (3+2). By these contacts the molecules are interconnected into endless chains. All polyhedra are deformed with the largest angle always accompanying the strongest bonds.

Intra- and intermolecular hydrogen bonds are formed in all of these three structures.

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