

**[s9.m2.p1] Crystal structures of *n*-octadecylammonium halides.** M. Rademeyer, D.G. Billing, G.J. Kruger. *Rand Afrikaans University, Johannesburg, South Africa.*  
Keywords: crystal chemistry, supramolecular compounds.

*n*-Alkylammonium halides have applications as surfactants, emulsifiers, lubricants, bactericides and detergents and they are commonly used as models to aid in the understanding of cell membrane structure.

These compounds crystallize as bilayers, that is, consisting of polar and non-polar layers. In the crystal the molecules are parallel, with the halide and ammonium ions in the polar layer interacting via hydrogen bonds. The hydrocarbon chains form the non-polar layers.

Results up to this day have shown that the lowest energy polymorph has an interdigitated structure. This means that the polar end of consecutive molecules in a layer point in opposite directions. Higher energy polymorphic forms are non-interdigitated. In these crystals the surface of the layers are formed by the same terminal groups.

Of interest is the alkyl chain conformation it has been observed as extend *trans* or kinked chains. In the case of *n*-octadecylammonium chloride<sup>1</sup> the kink is between the second and third carbon atoms, and for di-*n*-octadecylammonium bromide<sup>2</sup> the kink is between the third and the fourth carbon atoms. In addition anomalously long carbon-carbon bonds have been observed in this compound.

Structures of *n*-alkylammonium halides are compared with those reported in the literature and packing trends identified. Thermal investigations highlight the solid-solid phase transitions and thermal behavior of these bilayered compounds.

**[s9.m2.p2] Controlled host:guest ratio in inclusion compounds.** H. Su and L.R. Nassimbeni, *Department of Chemistry, University of Cape Town, Rondebosch 7701, Cape Town, South Africa.*

Keywords: inclusion, kinetics of desolvation, supramolecular crystallography.

It has been reported<sup>1,2,3</sup> that single crystals of inclusion compounds with varying host:guest ratios can be made by changing the crystallization conditions, i.e. temperature, cooling rate etc. The host 2,2'-dihydroxy-1,1'-binaphthyl(BINAP) formed two distinct inclusion compounds with guests 1,4-dioxane(DIOX) and dimethylsulfoxide(DMSO) respectively at different crystallization temperatures. X-ray structures analyses of these inclusion compounds [BINAP•1.5DIOX @60°C: P<sub>2</sub>/c; a = 8.938(1), b = 28.013(3), c = 9.137(1), β = 110.213(5); Z = 4. BINAP•3.5DIOX @25°C: P  $\bar{1}$ ; a = 10.322(1), b = 12.023(1), c = 13.432(1), α = 111.651(3), β = 91.955(3), γ = 90.716(3); Z = 2. BINAP•1DMSO @25°C: P<sub>2</sub>/n; a = 20.792(3), b = 8.883(1), c = 20.800(3), β = 105.115(5); Z = 8. BINAP•2DMSO @5°C: P<sub>2</sub>; a = 8.459(1), b = 8.927(1), c = 29.599(2) β = 92.907(4); Z = 4.] were reported. Their thermal stabilities were characterized by thermogravimetry(TG) and differential scanning calorimetry(DSC). The kinetics of desolvation of these compounds were studied and their activation energies were obtained.

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