Bilayers at the ILL

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Understanding properties of bilayers from a study of solid surfactants

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It has been known for a long time that adsorbed bilayers of *n*-alkyl trimethylammonium bromide surfactants, C_{*n*}TAB, at aqueous solution/hydrophilic solid interfaces are thin, much less than two extended hydrocarbon chains. These materials are bactericidal but the mechanism is not well-understood although differences in behaviour with chain length are established. For these reasons understanding factors that control their properties is important. We have studied the bulk phases of C₁₀TAB to C₁₈TAB systematically over a wide range of temperatures using X-ray diffraction and calorimetry. Small crystals can now be investigated routinely using modern laboratory equipment.[1] Common features in the structures are identified, with packing dominated by the co-ordination of the cationic head groups with bromide ions and interdigitation of the hydrocarbon chains. This arrangement provides an explanation for the thin adsorbed layers observed previously.[2] Molecular volumes and arrangement are comparable with structures of a number of different self-assembled amphiphiles. The alkyl chains are highly mobile and at high temperatures, a plastic phase is found for all materials with a transition enthalpy that is similar to the melting enthalpy of many long alkyl chains. The phase behaviour evidently depends on delicate balances of the various contributions to free energy. It is likely that the assembly and mobility of such surfactants is important in membrane penetration. Similar studies on other materials such as phospholipids are likely to yield further interesting results.

1. J. K. Cockcroft, *et al.* 'Understanding Structure and Dynamics of Cationic Surfactants from Studies of Pure Solid Phases' *PCCP* (2019), DOI: 10.1039/C9CP04486H.
2. G. Fragneto, *et al.* 'Neutron Reflection from Hexadecyltrimethylammonium Bromide Adsorbed on Smooth and Rough Silicon Surfaces' *Langmuir* 12, (1996), 6036-6043.

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