X-ray Reflectivity Study of Langmuir Films of Amphiphilic Monodendrons

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Introduction: Molecular and supramolecular monodendrons and dendrimers provide powerful building blocks for the construction of giant macromolecular and supramolecular systems with complex architecture and precise shape and functionality. Depending on the width of the aliphatic (peripheral) end and the apex (core), the monodendrons might be described as tapers, half-discs, discs, pyramids, cones, half-spheres, or spheres, resulting in columnar or cubic macroscopic lattices. The general principles determining molecular conformation at the air-water interface are still unclear. Is the molecular shape near the interface the same as it is in three dimensions? How important are the chemical functionalities of the different parts of the molecule? When monolayers are formed, are they flat, or composed of spherical, ellipsoidal, or cylindrical supramolecular structures?

Methods and Materials: We have used x-ray reflectivity and pressure-area isotherms to study a series of second- and third-generation monodendrons with hydrophobic $C_{12}H_{25}$ alkyl tails at the periphery and hydrophilic $COOHCO_2CH_3$ or crown ether groups in the core, one example of which is shown here. X-ray reflectivity profiles were analyzed via least-squares fits to a model incorporating a series of slabs and gaussian peaks.

Conclusions: We find that, with one exception, they are best described by a model in which the hydrophilic core is at or beneath the water surface, there is a low-density region just above the surface, and the alkyl chains form a high-density sub-layer above the surface with the chains directed perpendicular to the interface.

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References: W. J. Pao, M. R. Stetzer, P. A. Heiney, W.-C. Dong and V. Percec, submit. to J. Phys. Chem. B.