USES OF NEUTRON SCATTERING IN SUPRAMOLECULAR CHEMISTRY

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A major thrust in recent chemical research has been the development of supramolecular chemistry - broadly the chemistry of large *multicomponent* molecular assemblies in which the component structural units are held together by either covalent linkages or by a variety of weaker (non-covalent) interactions that include hydrogen bonding, dipole stacking, π-stacking, van der Waals forces and favourable hydrophobic interactions. Much of the activity in the area has been motivated by the known behaviour of biological molecules (such as enzymes). Thus molecular assemblies are ubiquitous in natural systems but, with a limited number of exceptions, have only recently been the subject of increasing investigation by chemists. A feature of much of this recent work has been its focus on molecular design for achieving complementarity between single molecule "hosts" and "guests".

The use of single crystal neutron diffraction coupled with molecular modelling and a range of other techniques to investigate the nature of individual supramolecular systems will be discussed. By way of example, in one such study the supramolecular array formed by co-crystallisation of 1,2-diaminoethane and benzoic acid has been investigated; the system self-assembles into an unusual layered structure composed of two-dimensional hydrogen bonded networks sandwiched between layers of edge-to-face stacked aromatic systems. The number of hydrogen-bond donors and acceptors is balanced in this structure.