

m42.o01**Molecular Recognition and Selectivity in Organic Clathrates**

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The use of inclusion compounds to separate a given guest from a mixture is one of the useful applications of host-guest chemistry. The process is dependent on the molecular recognition which occurs in the formation of the host-guest compound and may be studied in detail by crystallising a host compound, H, from a mixture of a pair of guests, A and B. The separation process may be presented by the equation $H(s, \alpha) + A(l) + B(l) \rightarrow H \infty A(s, \beta) + B(l)$ where H is the host compound in its non-porous α -phase, the apohost, A and B are liquid guests and the ensuing solid clathrate is $H \infty A$, the β phase. The process is imperfect, however, and the procedure has to be recycled a number of times in order to achieve a high level of separation. Competition experiments may be set up which allow us to measure the selectivity of a particular host H towards a given guest. The host compound H is dissolved in known mixtures of the guests A and B and the inclusion compound is allowed to crystallise. The crystalline clathrates are analysed and the ratio of A:B established by a suitable analytical method. The results are displayed as curves of X_B , the mole fraction of B in the liquid mixture, versus Z_B , the mole fraction of B in the crystals. In general four situations arise: a) The host displays no selectivity. b) The host preferentially enclathrates one guest over the whole concentration range. c) The host displays a selectivity which is concentration dependent and enclathrates the guest of greater concentration giving rise to a sigmoid curve. d) The host displays inverse selectivity, and captures the guest of minor concentration. Examples of all four selectivity results will be given and explained in terms of the crystal structures of the inclusion compounds and their lattice energies. The process has been extended to competition experiments carried out between three and four guests in a mixture.

m42.o02**Polymorphism and Structure-Property Relations in Molecular Crystals**

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There are two general strategies for investigating structure-property relations in materials:

1) Study a wide variety of materials and their properties in order to isolate the particular factors relating particular structural features to desired properties, or 2) Eliminate as many structural variables as possible to isolate the relationship between a particular property and the structures associated with it. The second approach is particularly efficient and effective if appropriate polymorphic systems are chosen for study, since all molecular chemical and substitutional variables are necessarily eliminated, the only remaining variable among polymorphs being the difference in crystal structure, with possible variations between molecular conformation in the various structures. This strategy has been applied successfully in the study of a variety of properties, both bulk properties and molecular properties. The study of the structure-property relations in polymorphic structures provides an additional incentive. Frequently the different polymorphs are obtained under different crystallizing conditions, which can also yield information on how to achieve certain structures with desired properties or avoid structures with undesired properties. A number of examples will be presented to demonstrate the strategy and the information that may be obtained by utilizing polymorphs to study structure-property relations.