

PS06.06.03 SEPARATION OF CLOSE ISOMERS BY ENCLATHRATION. A. Horne^a, M. R. Cairns^a, L. R. Nassimbeni^a, K. Okuda^b and F. Toda^b ^aDepartment of Chemistry, University of Cape Town, Rondebosch 7700, South Africa ^bDepartment of Applied Chemistry, Faculty of Engineering, Ehime University, Matsuyama 790, Japan

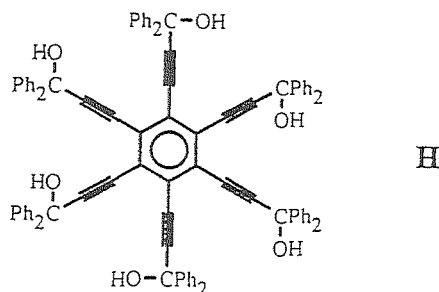
The separation of close isomers by clathrate formation is industrially important because it is simple, efficient and is not energy intensive. The process relies on molecular recognition between host and guest molecules, and typically consists of dissolving an appropriate host compound in a mixture of two or more guests, allowing the formation of a crystalline inclusion compound which is enriched with respect to a particular guest. The inclusion compound is filtered and the enriched guest released by gentle warming, so that the host compound can be recycled. Depending on the selectivity of the process, separation of the targeted guest of >90% is usually achieved in at least three cycles¹⁻².

1. D. R. Bond and F. Toda, *Acta Crystallogr., Sect. C*, 1991, **47**, 348.
2. I. Goldberg, Z. Stein, K. Tanaka and F. Toda, *Chem. Lett.*, 1987, 1617.

PS06.06.04 SELECTIVE INCLUSION OF KETONE BY A SEXIPEDAL HOST. Katherine L. Gifford Nash^a, Susan A. Bourne^a, Fumio Toda^b. a) Department of Chemistry, University of Cape Town, Rondebosch, 7700, South Africa. b) Department of Applied Chemistry, Faculty of Engineering, Ehime University, Matsuyama 790, Japan.

Hexakis(3-hydroxy-3,3-diphenyl-2-propenyl)benzene (**H**) has proved to be a very versatile host including a number of small organic molecules via hydrogen bonding. Inclusion compounds of **H** have been found to form in various host:guest ratios, often considerably richer in guest than is usually observed for organic hosts. It includes a number of guests with carbonyl functions, for example methyl ethyl ketone (1:3), diethyl ketone (1:2) and cyclohexanone (1:5); as well as guests such as diethyl ether (1:2) and 1,4-dioxane (1:5).

However, on crystallization from 1,3-dioxolane, **H** selectively included a trace amount of 1,3-dioxolan-2-one from the solution. This ketone complex was characterised by single crystal diffraction, thermal analysis, nuclear magnetic resonance spectroscopy, and mass spectroscopy.



PS06.06.05 WHAT MAKES CLATHRATES STABLE? Kersti Hermansson, Dept. of Chemistry, Uppsala University, Box 531, S-75121 Uppsala, Sweden

The β -quinol clathrate crystal is built up of approximately spherical cages, about 4 Å in diameter. This cage structure is stable only when guest molecules are trapped within the cages. Without guests, another modification of quinol, the α -form, is the most stable structure. The experimentally measured enthalpy difference for the process α -quinol \rightarrow β -quinol is only 0.6 kJ/mol. The enthalpy change for the inclusion of guest molecules into the β -quinol cages has been measured to -25 to -60 kJ/mol, depending on the type of guest molecule.

Many experimental studies of β -quinol inclusion compounds have been reported. The preferred sites and the motion of the guest molecules in the cages have been investigated. No ab initio calculations of these crystalline compounds have yet been presented.

This paper presents results from crystal-orbital calculations of different β -quinol inclusion compounds at the Hartree-Fock and Hartree-Fock + DFT levels. Optimized structures, clathrate formation energies and the much debated role of the guest-guest interactions will be presented.

PS06.06.07 THE STRUCTURAL ASPECTS OF DURENE-THIOUREA INCLUSION COMPLEX. Marfo-Owusu Emmanuel, Department of Chemistry, University of Transkei, P/Bag X1, Umtata, Eastern-Cape province, Republic of South Africa

The crystal structure of durene-thiourea [$2C_{10}H_{14} \cdot 9SC(NH_2)_2$] has been determined by X-ray diffraction method. The structural aspect of this inclusion complex with respect to the crystal structure, host cavity shape and guest cavity shape after the monoclinic deformation is attributed to the distorted lattice of the guest (durene) molecule.