Supported bimetallic particle catalysts (with particle sizes a few nanometres) are being increasingly used in heterogeneous catalysis due to their enhanced selectivity introduced by changes in their surface and electronic structure. Cu-Pd supported on carbon is of interest to commercial methanol synthesis reactions. Using an in-situ 1 MeV EM fitted with a gas reaction cell, reactions in H₂ and CO are monitored and different sintering behaviour has been observed. Surface defect layers of up to only a few angstroms in the reacted catalysts have been observed by high resolution microscopy using a JEOL 200CX and a JEOL 4000EX HR-EMs. Particle structures are identified by convergent beam diffraction patterns. High precision microanalysis with probe sizes 3-5 nm has indicated preferential surface enrichment of Pd. The surface structure information is critical to the understanding of chemisorption of the synthesis gases and therefore, to activity. Based on the microanalysis and HR-EM results, calculations of these complex images have been carried out using 256x256 FFTs (array) in the multislice programmes. The calculations have been performed for both possible models: Pd at the surface and Cu at the surface as a function of thickness and defocus. The results have shown a marked difference in the image contrast between the two models and simulations using Pd-edge are in agreement with the experimental data. It is shown for the first time that even a monolayer coverage of a particular species on the nanometre size particles can be distinguished.

**04.5-1 MOLECULAR SEPARATIONS BY LATTICE INCLUSION**

*By I. Goldberg and F. Toda*

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This presentation is concerned with structural design and characterization of a series of new host-guest compounds which can be used for isolation and optical resolution of material by lattice-inclusion type complexation. Lattice inclusion selectivity and guest discrimination has been observed in coordinato-clathrates formed by several functional hosts such as N,N'-dipropyliurea (DTU), 1,1-dip(4-hydroxyphenyl)cyclohexane [DHC] and 1,1-bis(2-naphthyl)ethane [BNL]. Lattice inclusion is a versatile property of selective complexation towards guests of different functionality and molecular shape (Mart, Lin and Goldberg, H.C. Ørsted Inst. of Phys. Chem., 277-286). The DHC host has been applied successfully to separations of cresols from a cresol mixture obtained from coal tar. Selectivity studies showed preferential complexation of this host with m-cresol > p-cresol > phenol > o-cresol, leading to 98.5% pure isolation of m-cresol. The two pairs of coordination compounds are resolved separately by a simple extraction with ether. It has been shown for the first time that even a monolayer coverage of a particular species on the nanometre size particles can be distinguished.

**04.5-2 CRYSTAL STRUCTURES OF HEXAKIS(2,6-0-METHYL)-α-CYCLODEXTRIN INCLUSION COMPLEXES**

*By Kazuaki Harata, Research Institute for Polyomers and Textiles, 1-1-4 Yatate-Higashi, Tsukuba, Ibaraki 305 Japan*

Hexakis(2,6-di-0-methyl)-α-cycloextrin (diastereomeric α-CDx), which is expected to have an intramolecular cavity larger than that of parent α-CDx, forms inclusion complexes in the solid state and in solution. We have determined the crystal structures of three hexamethyl-α-CDx complexes to investigate the effect of methylation on the macrocyclic conformation and the guest-host interaction. Crystallographic data are as follows:

1. α-Propanol complex: C₅H₁₂O₂·C₅H₁₂O₂ H₂P₂, Z=2, a=11.363(2), b=10.686(1), c=21.447(2), β=106.06(1)°, R=0.058, (2) iodine complex: C₅H₁₂O₂·H₂O·P₂, Z=2, a=14.124(2), b=10.667(2), c=21.463(2), β=106.29(1)°, R=0.077, (3) 3-iodopropionic acid complex: C₅H₁₂O₂·I₂, Z=4, a=0.084(3), a=0.084(3), a=0.084(3), b=15.569(3), b=15.569(3), b=15.569(3), c=8.093.

The hexamethyl-α-CDx molecule has a round shape which is maintained by intramolecular 0(3)-H···0(2) hydrogen bonds. 3-Iodopropionic acid is located at the center of the host cavity, while iodine and 1-propanol molecules are shifted toward the wider 0(2), 0(3) side from the center of the cavity. Dimethyl-α-CDx molecules are arranged to form a typical "cage" type packing in the crystal.

**04.5-3 CHIRAL DISCRIMINATION AND THE CRYSTAL STRUCTURES OF PAIRS OF DIASTEREOISOMERIC SALTS**

*By Rine Larsen. Department of Physical Chemistry, H.C. Ørsted Institute, University of Copenhagen, Denmark.*

A commonly used method for separation of enantiomers in a racemic mixture is to add a suitable chiral reagent, that reacts (precipitates) with the racemate, e.g. R,R-tartaric acid is a widely used reagent for the resolution of optically active amines. The two different diastereoisomeric salts that may result from the reaction can differ so much in their relative solubilities that an almost quantitative separation of the enantiomers is achieved. To investigate the chiral discrimination, we have limited our studies to systems where the two diastereoisomeric salts have identical composition.

The crystal structures have been determined for pairs of diastereoisomeric salts. As this is the aim to relate the differences between the intermolecular interactions in the structures to the difference in solubility, we have limited our studies to systems where the two diastereoisomeric salts have identical composition. The crystal structures have been determined for the salts obtained when enantiomers of the organic amines 1-aminopropanol, 1-aminobutanol and 1-(2-pyridyl) ethyamine are resolved as hydrogenatecarbines and for two pairs of coordination compounds. A careful examination of the intermolecular interactions in these compounds shows that both hydrogen bonds and non-bonded interactions are important for the crystal packing. A qualitative comparison between the intermolecular interactions in equivalent diastereoisomeric salts showed that the number and the strength of the hydrogen bonds in the structures are very similar and that the difference in solubility mainly arise to differences in the non-bonded interactions. The results will be related to the thermodynamics of the resolution process.