

s9.m2.o3 **Dynamic Aspect of Lattice Inclusion Complexation Involving Phase Change.** Y. Aoyama, *Institute for Fundamental Research of Organic Chemistry, Kyushu University, Fukuoka 812-8581, Japan*

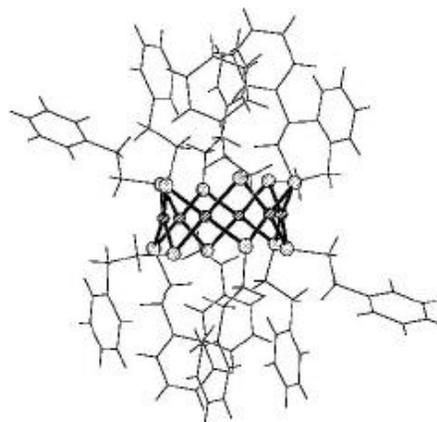
Keywords: crystal engineering, phase change, network.

When immersed in an aqueous solution of alcohol or alkyl acetate as a guest, anthracenebisresorcinol **1** as a hydrogen-bond networked solid host extracts two mols of the guest together with 3-8 mols of water. The binding isotherm shows a sharp threshold guest concentration characteristic of host/adduct phase-transition. The threshold concentrations as a measure of affinities are highly dependent on the hydrophobicities of the guests. Host **1** also catalyzes the Diels-Alder reaction of acrolein and 1,3-cyclohexadiene in an aqueous environment. The preserved 1:2 (host-to-guest) stoichiometry, spectroscopic evidence ($\Delta\nu_{C=O}$), guest-desorption behaviors, and X-ray powder-diffraction studies indicate that host-guest hydrogen-bonding in collaboration with apolar interactions is responsible for the selective guest-binding and catalysis under the present aqueous conditions.

s9.m2.o4 **A Study of Molecular Motions in a Cyclic Hexanuclear Nickel Thiolate by NMR and X-ray Diffraction Techniques.** A.H. Mahmoudkhani^a and V. Langer^b, *a) Department of Inorganic Chemistry, Göteborg University, SE-41296 Göteborg, Sweden and b) Department of Environmental Inorganic Chemistry, Chalmers University of Technology, SE-41296 Göteborg, Sweden.*

Keywords: molecular interactions, supramolecular compounds.

Metal thiolates, including nickel thiolates, are a rich class of compounds and are relevant to the coordination of metal ions by cysteine in biological systems and metal sulfide catalysis. They are also interesting as self-assemblies of the molecular clusters. Cyclic polynuclear nickel thiolates are built up from a polygonal cluster of NiS₄ units linking together by thiolate ligands. There are several practical problems associated to the structural characteristics of these compounds namely the high electron density in the core of the molecular cluster and dynamic processes associated to the molecular motions of the thiolate ligands both in solution and in solid state. We have recently developed an efficient method for X-ray diffraction data collection using area detectors that overcomes the first problem mentioned above. Low-temperature crystallography seems to be a simple remedy for the second problem with a risk of cracking the crystals, possible phase transitions or difficulties to resolve diffraction spots.



In this study we wish to report the molecular motions of hexakis[di- μ -(2-phenylethanethiolato)nickel] in solution and solid state as seen by NMR and X-ray diffraction techniques. The crystal structure of the compound and thermal displacement parameters have been studied as a function of temperature between 183 and 323 K. Results from ¹H-NMR analysis in solution are in accordance with the data from diffraction analysis.