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Index Abstracts

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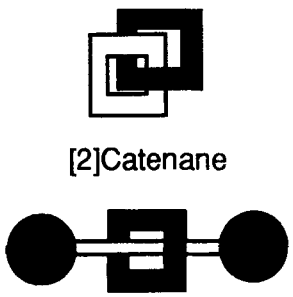
Index Abstracts

The efficiency of the self-assembly of a range of interlocked molecular compounds has been studied as a function of the recognition sites present in the molecule that make up the molecular assemblies. While constitutional changes have opened up avenues to polycatenanes, steric and electronic changes associated with the recognition sites have provided an opportunity to investigate and control translational isomerism.



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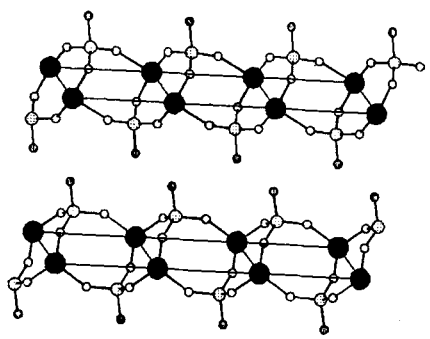
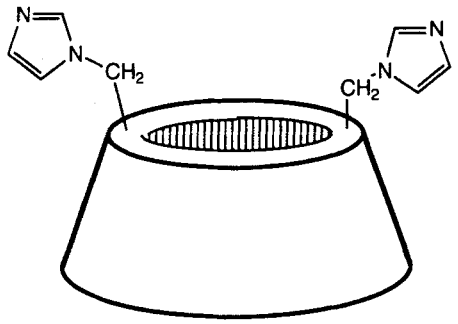
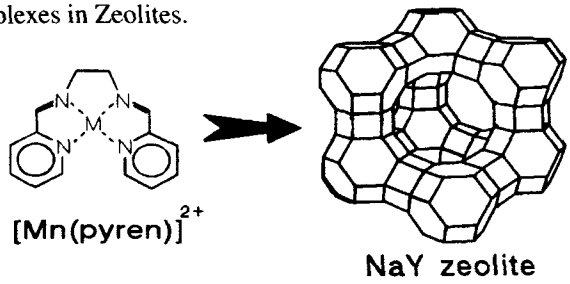
After a brief account on previous results obtained in this Laboratory in the field of layered and pillared α and γ zirconium phosphonates, the perspectives for a development of a "molecular recognition" in porous and in layered solids are examined.



In the final structure of an enzyme-substrate complex, or of a related molecular complex, the two components may fit together in a lock and key relationship, but flexibility is often needed in the binding process.



Catalytic and Physico-chemical Properties of New Schiff base Complexes in Zeolites.



D. E. De Vos, P. P. Knops-Gerrits, D. L. Vanoppen, and P. A. Jacobs

Catalytic and physico-chemical properties of new schiff base complexes in zeolites

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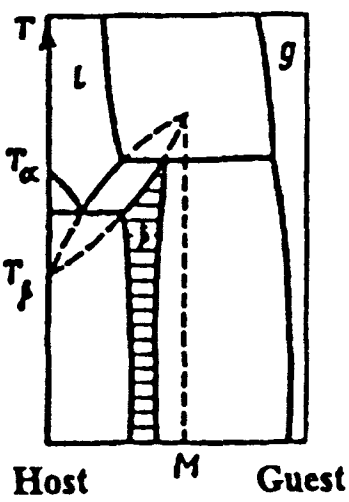
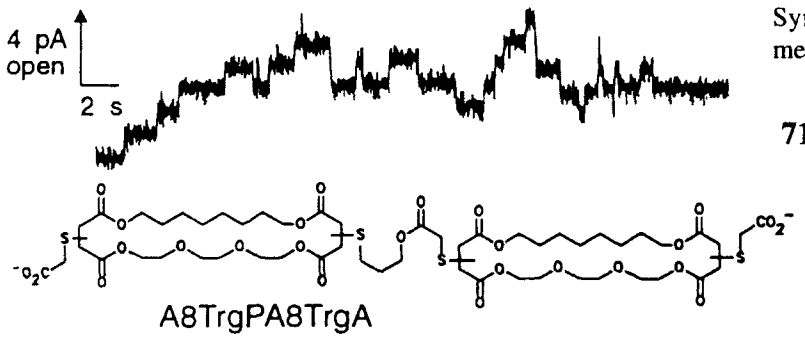
Different stoichiometric interrelations from solid solutions on the basis of the stable host modification to constant composition clathrates via classic clathrates of variable compositions are illustrated in the guest-host systems and summarized picture of this phenomenon is discussed.



Yuri A. Dyadin

On the stoichiometry of clathrates

Simple linear pore-formers give controlled ion-selective channels, while more complex structures give irregular bursts of activity.



Thomas M. Fyles, Daniela Heberle, Wilma F. Van Straaten-Nijenhuis and Xin Zhou

Synthetic ion transporters in bilayer membranes

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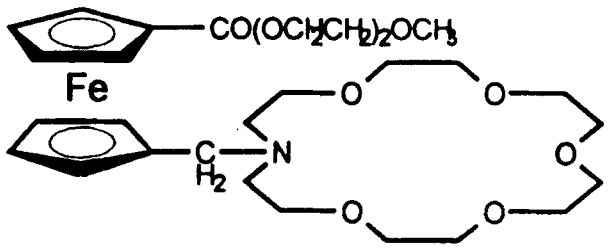
Ferroceynl lariat ether complexing agents have been prepared.

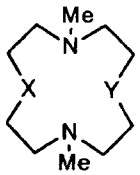


Chensheng Li, Mara Tsesarskaja, and George W. Gokel

Ferrocene as a molecular building block in lariat ethers and other complexing agents

79-85

Two general methods of the synthesis of diazacoronands.

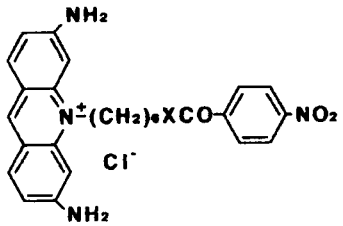


J. Jurczak, P. Lipkowski, T. Stankiewicz and Z. Urbańczyk-Lipkowska

Diazacoronands - synthesis, structure and inclusion properties

87-94

DNA binding and DNA cleavage specificities of two novel classes of synthetic DNA breakage agents.



1a X = O
1b X = NH

Reiko Kuroda, H. Tanaka, H. Satoh, M. Shinomiya, T. Amagai and M. Furubayashi

Intelligent compounds which read DNA base sequences

95-102

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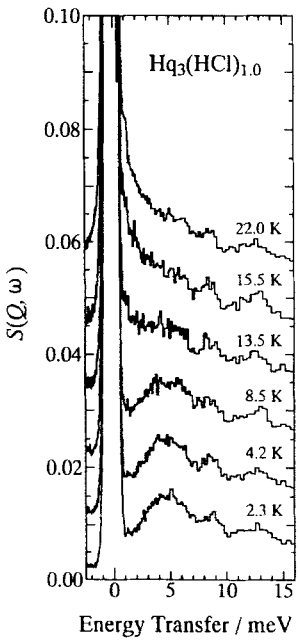
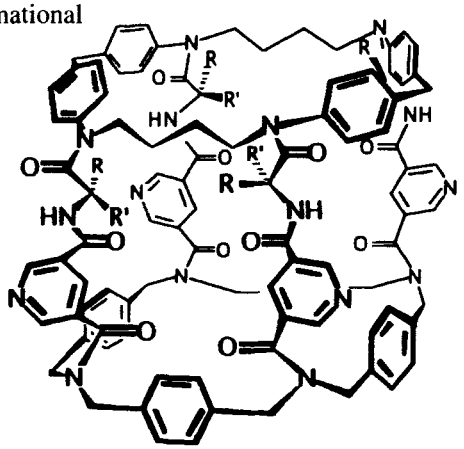
Low temperature properties of clathrate compounds of hydroquinone and thiourea and of clathrate hydrates are discussed using experimental results from calorimertry, neutron scattering and nuclear resonance experiments.



Takasuke Matsuo and Osamu Yamamuro

Phase transitions in some clathrate compounds

Novel cage-type cyclophanes, which are constructed with two macrocyclic skeletons and four chiral bridging components, have been synthesized. The present cage-type hosts performed size- and shape-sensitive molecular discrimination toward nonionic fluorescent guests of various bulkiness due to their rigid conformational framework.



Osamu Hayashida, Kazuya Ono, and Yukito Murakami

Size- and shape-sensitive molecular discrimination by cage-type cyclophanes in aqueous media

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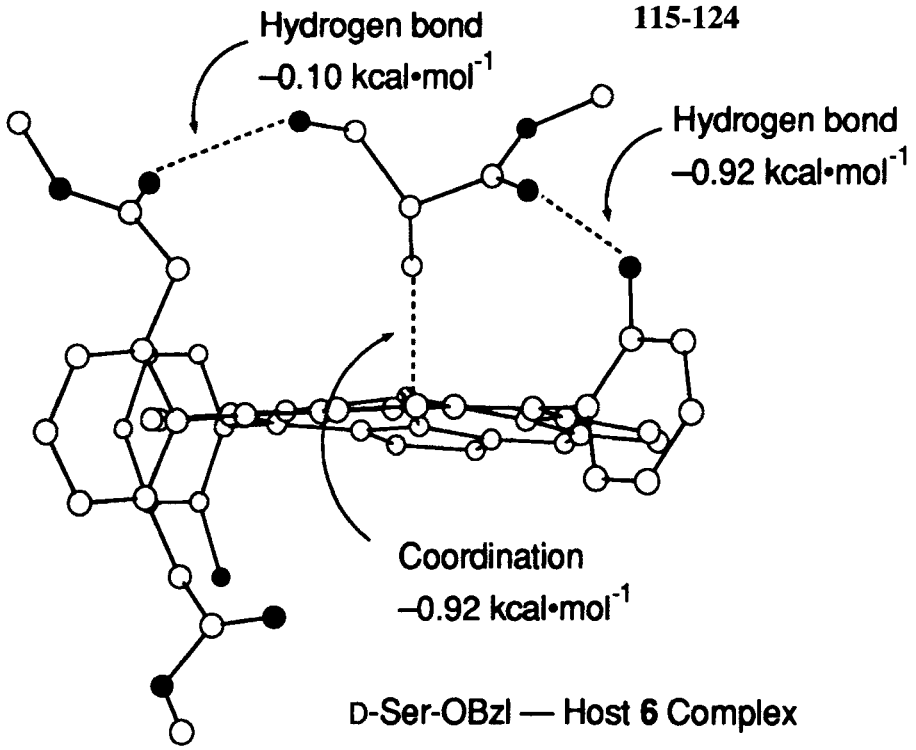
Preparation and recognition ability of new chiral porphyrins with multi-point recognition groups are described. Thermodyanmic analysis of multi-point recognition is summarized. Application of this approach to chiral recognition by porphyrin hosts is then reported.

Hisanobu Ogoshi, Tadashi Ema, Yusuke Kato, Tadashi Mizutani and Yasuhisa Kuroda

Molecular recognition: New chiral metalloporphyrins as receptor models



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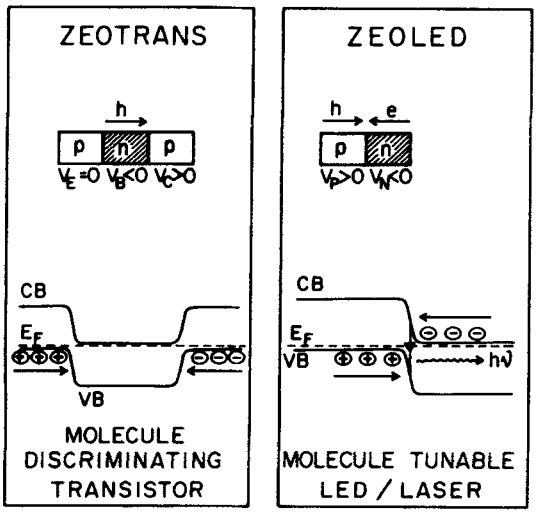
A novel class of flexible open frame-work nanoporous tin(IV) chalcogenide electronic materials is described.

Geoffrey Alan Ozin

Microporous and mesoporous electronic materials: flexible open-framework nanomaterials for molecular recognition, towards the electronic nose

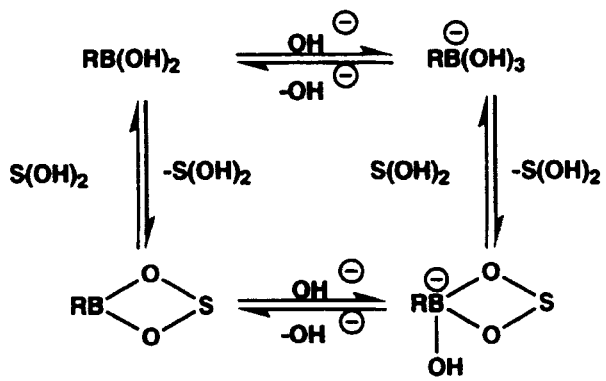


Monte Carlo methods are effective in docking ligands, ranging in size from molecular fragments up to proteins, to protein targets of known 3D structure.

R. J. Read, T. N. Hart, M. D. Cummings and S. R. Ness

Monte Carlo algorithms for docking to proteins

A various kind of boronic-acid-appended sugar receptors were designed.



Tony D. James, K. R. A. Samankumara Sandanayake and Seiji Shinkai

Recognition of sugars and related compounds by "reading-out" -type interfaces

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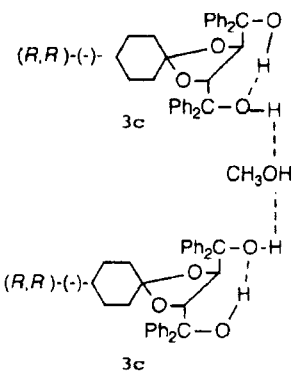
Host-guest solid state chemistry and distillation afford resolution.



Fumio Toda

Chiral lock and chiral key in inclusion crystals

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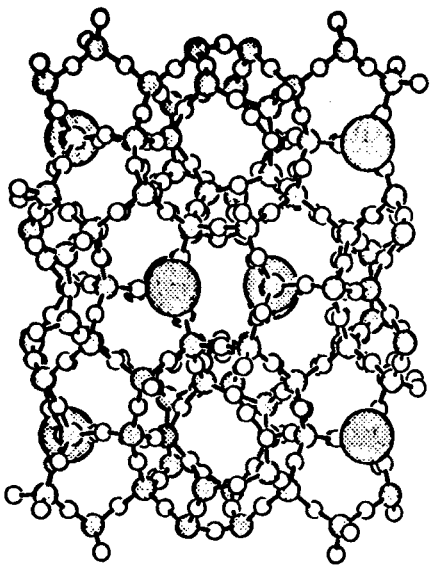
The mechanism for the novel structural memory effect is investigated using clathrasil dodecasil as a model system.

John S. Tse and Dennis D. Klug

Reversible amorphization and structural memory effect in clathrasil dodecasil-3c

165-170



1 bar

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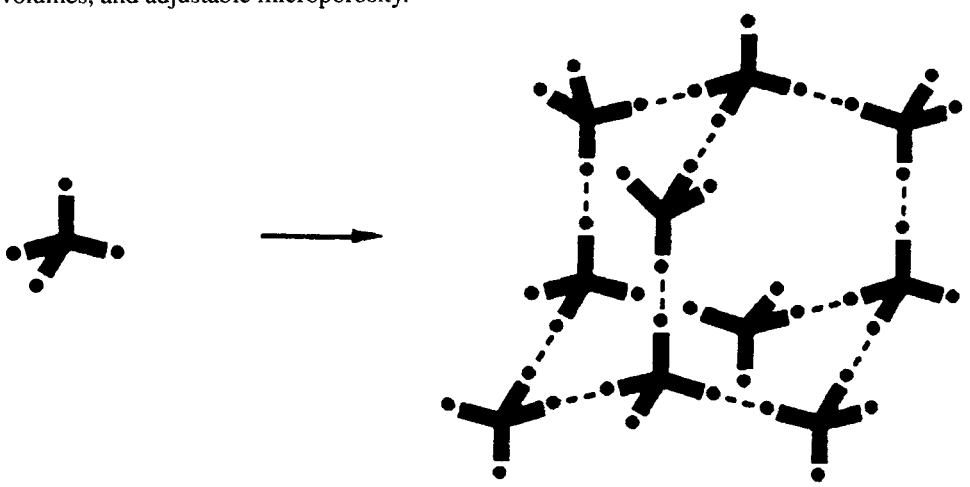
The strategy of molecular tectonics can be used to build a wide variety of ordered three-dimensional organic networks with some of the desirable properties of zeolites and related inorganic materials, including high structural integrity, potentially large void volumes, and adjustable microporosity.

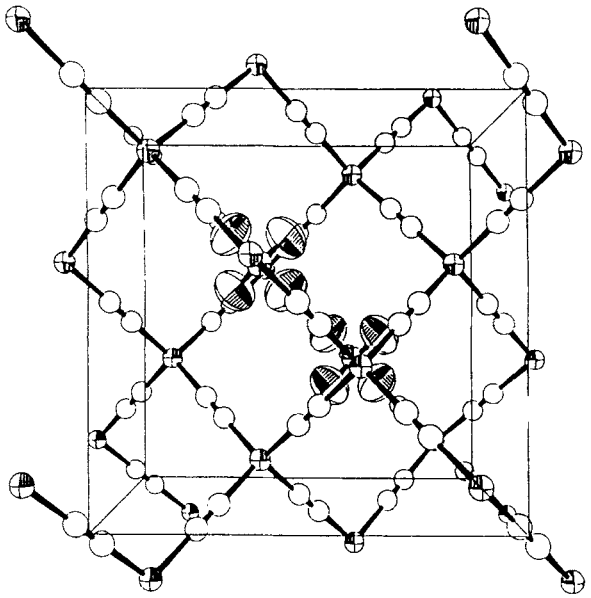
Dan Su, Xin Wang, Michel Simard and James D. Wuest

Molecular tectonics

171-178



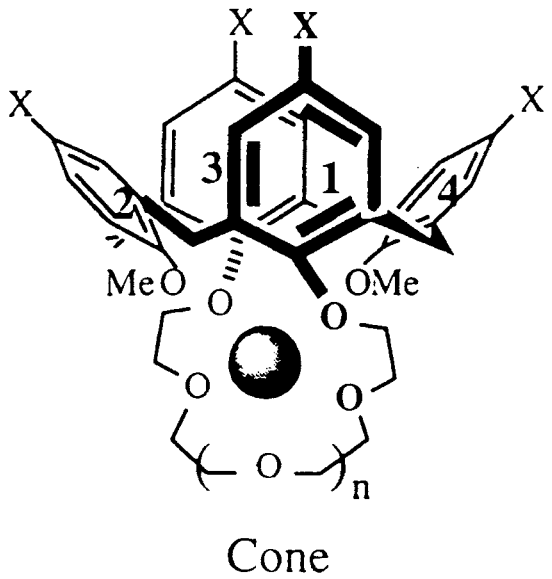
The structural similarity between $Cd_{\chi}(CN)_{\gamma}$ and $Si_{\chi}O_{\gamma}$ in the $A_{\chi}B_{\gamma}$ composition can be utilized in developing mineral-like supramolecular structures.



Toschitake Iwamoto, Shin-ichi Nishikiori and Takafumi Kitazawa

Mineralomimetic chemistry of cyanometallates

Molecular dynamics and free energy calculations are presented for calix[4] crown in water and the gas phase.



Cone

G. Wipff and M. Lauterbach

Complexation of alkali cations by calix[4] crown ionophores: conformation and solvent dependent Na^+/Cs^+ binding selectivity and extraction: MD simulations in the gas phase, in water and at the chloroform-water interface

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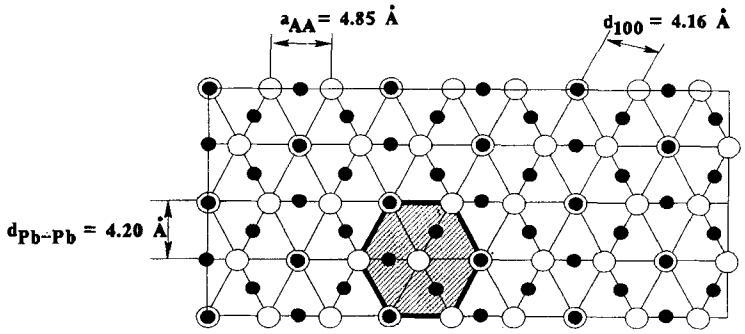
PbS has been epitaxially grown under arachidic acid (AA) monolayers due to the overlap between Pb^{2+} ions and AA headgroups; O = AA headgroup, • = Pb^{2+}, and ◉ = Pb^{2+} and AA headgroups. A unit cell is highlighted by the dotted area which is enclosed by heavy lines.

Janos H. Fendler

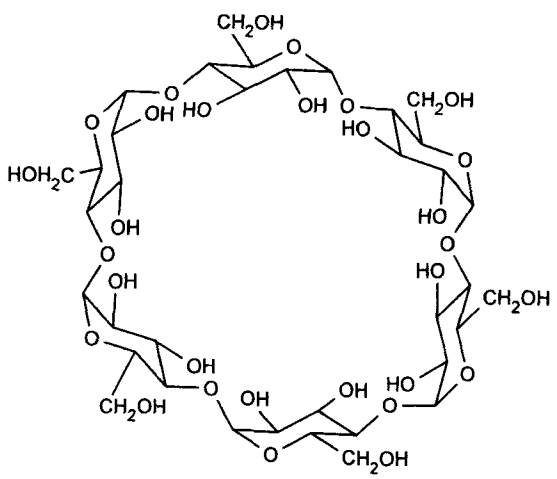
Expitaxial growth of size-quantized semiconductor particles at monolayers



Generally we can not fit a "guest" to a cyclodextrin (CD), but we can select (or even synthesize by modifying the CD-structure) a better fitting -host- for a given guest.

J. Szejtli

Selectivity/structure correlation in cyclodextrin chemistry



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