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Index Abstracts

Molecular recognition behavior of eight chromophore-modified cyclodextrins with a series of aliphatic alcohols and carboxylic acid has been investigated by using spectropolarimetric or spectrofluorometric titration.

Yu Liu, Chang-Cheng You, Takehiko Wada and Yoshihisa Inoue

Molecular Recognition of Aliphatic Alcohols and Carboxylic Acid by Chromophoric Cyclodextrins

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p-Picolinio m-Toluidino 8-Quinoly 2-Naphthylamino

Discrimination of chiral amines by dimethyldiketopyridino-18-crown-6 (1) is studied by free energy perturbation (FEP) and moleculardynamics (MD) methods.

One-Sun Lee, Sungu Hwang and Doo Soo Chung

Free Energy Perturbation and Molecular Dynamics Simulation Studies on the Enantiomeric Discrimination of Amines by Dimethyldiketopyridino-18-Crown-6

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The nature of the CH- π (aromatic) interactions, which stabilise the complexes between calix[4]arenes and guest the type CH₃X and CH₂XY, was investigated in the solid state. The geometrical parameters which define the shape of the host, the position and the orientation of the guest in their complexes indicate the different nature of these interactions in the two types of complexes.

Arturo Arduini, Francine F. Nachtigall, Andrea Pochini, Andrea Secchi, and Franco Ugozzoli

Calix[4]Arene Cavitands: A Solid State Study on the Interactions of their Aromatic Cavity with Neutral Organic Guests Characterised by Acid CH_3 or CH_2 Groups





The complexation with sodium perchlorate induced effectively the conformational change of 1b into a slipped face-to-face structure.

Shigeyuki Yagi, Ryuhei Yamada, Norihiro Tsuji, Shinji Murakami and Toru Takagishi

Conformational Control of a Polyether-Linked Porphyrin Dimer Induced by Complexation with a Sodium Cation



Circular dichroism, fluorescence, and NMR spectroscopic studies were performed to elucidate the conformations of anilino- and *m*-Toluid-ino- β -cyclodextrins in aqueous solution, and the binding constants of both modified β -cyclodextrins with various aliphatic alcohols were obtained by spectropolarimetric titrations.

Yu Liu, Chang-Cheng You, Mieko Kunieda, Asao Nakamura, Takehiko Wada and Yoshihisa Inoue

Molecular Recognition Studies on Supramolecular Systems. 29. Anilinoand *m*-Toluidino- β -Cyclodextrins: Structural and Conformational Analyses and Molecular Recognition of Aliphatic Alcohols

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In the presence of silver(I), tetracyanocalix[4]arene assembles into a one-dimensional coordination polymer. The crystal structure of the free ligand is also presented.

Eric Elisabeth, Leonard J. Barbour, G. William Orr, K. Travis Holman and Jerry L. Atwood

Synthesis and structure of a one dimensional coordination polymer based upon tetracyanocalix[4]arene in the cone conformation

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We have demonstrated that cerium(IV) double decker porphyrins which have more than two pairs of 4-pyridyl groups(3b~3d) show a high positive allosteric effect through the hydrogen-bonding interaction between 4-pyridyl pairs and dicarboxylic acids.

M. Ikeda, M. Takeuchi, A. Sugasaki, A. Robertson, T. Imada, and S. Shinkai

Strong Positive Allosterism which Appears in Molecular Recognition with Cerium(IV) Double Decker Porphyrins: Correlation between the Number of Binding Sites and Hill Coefficients

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