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Index Abstracts

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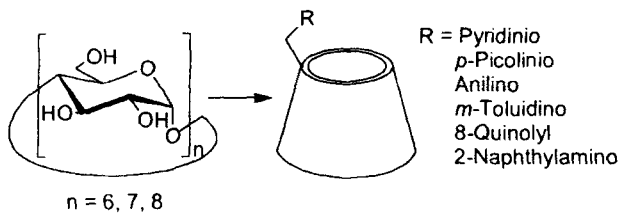
Index Abstracts

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

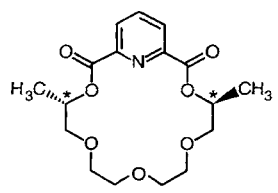
Molecular Recognition of Aliphatic Alcohols and Carboxylic Acid by Chromophoric Cyclodextrins



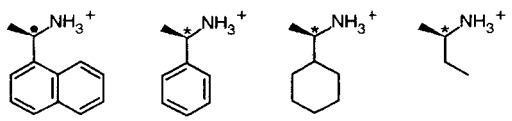
Discrimination of chiral amines by dimethyldiketopyridino-18-crown-6 **(1)** is studied by free energy perturbation (FEP) and moleculardynamics (MD) methods.

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

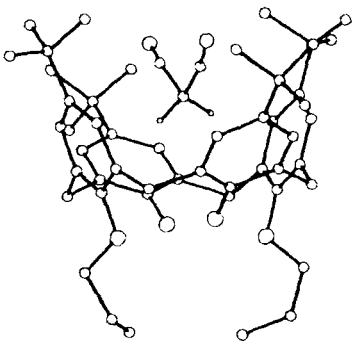


1

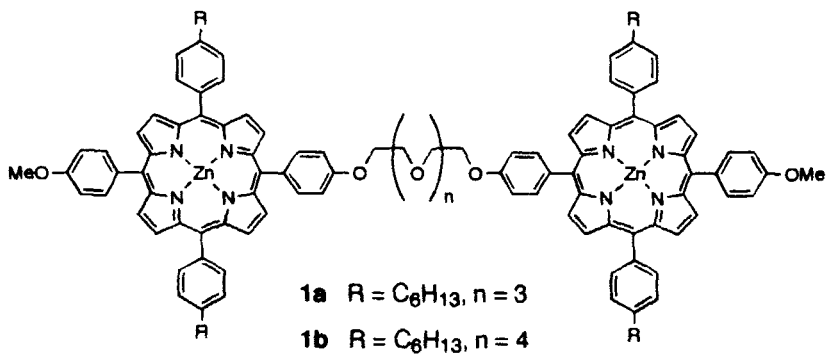


2 **3** **4** **5**

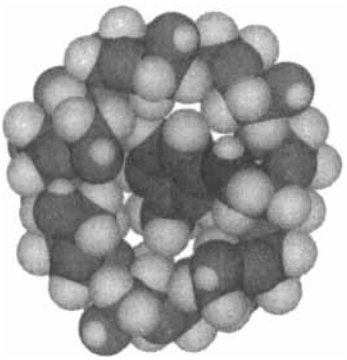
The nature of the CH-π(aromatic) interactions, which stabilise the complexes between calix[4]arenes and guest the type CH_3X and CH_2XY, was investigated in the solid state. The geometrical parameters which define the shape of the host, the position and the orientation of the guest in their complexes indicate the different nature of these interactions in the two types of complexes.



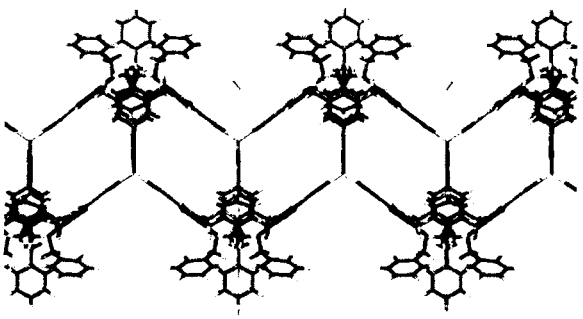
The complexation with sodium perchlorate induced effectively the conformational change of 1b into a slipped face-to-face structure.



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



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.

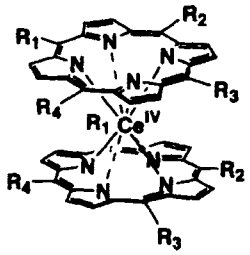


We have demonstrated that cerium(IV) double decker porphyrins which have more than two pairs of 4-pyridyl groups(3b~3d) show a high positive allosteric effect through the hydrogen-bonding interaction between 4-pyridyl pairs and dicarboxylic acids.
*

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

321 – 345



3a' R_1= Py R_2,R_3,R_4 = Ph
3a :R_1= Py R_2,R_3,R_4 = An
3b$_p$ R_1,R_2 = Py R_3,R_4 = An
3b$_d$ R_1,R_3 = Py R_2,R_4 = An
3c :R_1,R_2,R_3 = Py R_4 = An
3d :R_1,R_2,R_3,R_4 = Py