























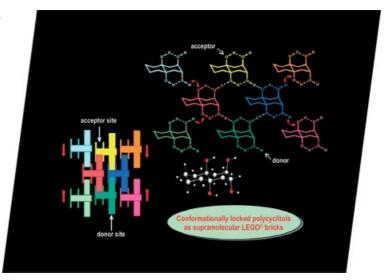




The EUChemSoc Societies have taken the significant step into the future by merging their traditional journals, to form two leading chemistry journals, the European Journal of Inorganic Chemistry and the European Journal of Organic Chemistry. Three further **EUChemSoc Societies (Austria,** Czech Republic and Sweden) are Associates of the two journals.

COVER PICTURE

The cover picture shows, schematically, the manner in which a conformationally locked polycyclitol can be thought of as a LEGO® brick in the supramolecular world. This analogy manifests during the self-assembling process by involvement of intermolecular H-bond donors and acceptors engendered in preordained positions through the rigid trans-decalin framework and intramolecular O-H···O hydrogen bonding between the 1,3-diaxial OH groups. Details are discussed in the article by G. Mehta et al. on p. 423ff.



MICROREVIEW

Carbohydrate Carbocyclization

R. Madsen* 399-415

Synthetic Strategies for Converting Carbohydrates into Carbocycles by the Use of Olefin Metathesis

Keywords: Carbocycles / Carbohydrates / Metathesis / Olefination / Total synthesis

Recent advances in the use of RCM for converting carbohydrates into carbocycles are reviewed, including methods for the syn-

thesis of dienes, RCM reactions and application to natural product synthesis.

SHORT COMMUNICATIONS

1,10-Phenanthroline Chemistry

O. Moudam, F. Ajamaa, A. Ekouaga,

H. Mamlouk, U. Hahn, M. Holler,

R. Welter, J.-F. Nierengarten* 417-419

A New Synthetic Route for the Preparation of 1,10-Phenanthroline Derivatives

Keywords: 1,10-Phenanthroline / Organolithium reagents / Cleavage reactions / Heterocycles

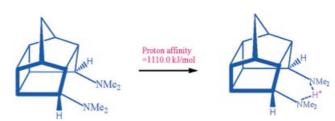
Benzylated dihydrophenanthroline derivatives have been prepared to modify the chemical reactivity of the phenanthroline backbone.

Proton Sponges

A. Singh, B. Ganguly* 420-422

DFT Studies toward the Design and Discovery of a Versatile Cage-Functionalized Proton Sponge

Keywords: Basicity / Cage compounds / DFT calculations / Design



Superduper: According to DFT calculations, pentacyclo[5.4.0.0^{2,6}.0^{3,10}.0^{5,9}]-undecane (PCU) derivatives have been predicted as superorganic bases. The new mo-

lecular framework (PCU) is versatile in terms of anchoring different functional groups to achieve high basicities in both the gas and solvent phases.



FULL PAPERS



That conformational locking of hydroxyl groups in polyols lends enhanced predictability to the molecular packing of such molecules in the solid state has been revealed through a comparison between the

qualitatively proposed models of supramolecular aggregation and experimentally observed crystal structures in three polycyclitols, which have been specially crafted on a rigid *trans*-decalin backbone.

Crystal Engineering

G. Mehta,* S. Sen, S. S. Ramesh 423–436

Crystal Structures of Conformationally Locked Cyclitols: An Analysis of Hydrogen-Bonded Architectures and their Implications in Crystal Engineering

Keywords: Crystal engineering / Conformational locking / Cyclitols / Fused-ring systems / Hydrogen bonds

The intramolecular amidation reaction of a series of *N*-aryl-substituted unsaturated amides mediated by the hypervalent iodine reagent PIFA is studied. The cyclization process takes place with simultaneous generation of a hydroxy group at the terminal position of the original double bond.

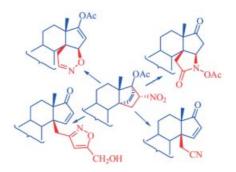
Synthetic and mechanistic study starting from 22 different substrates

Intramolecular C-N Bond Formation

On the Phenyliodine(III)-Bis(trifluoroacetate)-Mediated Olefin Amidohydroxylation Reaction

Keywords: Hypervalent iodine / Pyrrolidines / *N*-Acylnitrenium / PIFA / Cyclization

The Diels–Alder adduct of a steroidal 14,16-diene and nitroethylene can be reduced with $TiCl_3$ to give an oxazine, whereas its treatment with Lewis acids leads to a derivative of the cyclic hydroximic acid. The 16α -nitro cycloadduct suffers a weakbase-induced cleavage of the C(16)-C(17) bond, releasing the nitrile oxide intermediate, which can be trapped by a dipolarophile or reduced with triphenylphosphane.



Bridgehead Cleavage Reactions

Synthesis of 3-Methoxy- 16α -nitro-14,17-ethenoestra-1,3,5(10)-trien- 17β -yl Acetate and Fragmentation-Mediated Pathways to $14\beta,15\beta$ -Fused *N*-Heterocycles and 14β -Functionalised Alkyl Derivatives

Keywords: Steroids / Nitrogen heterocycles / Cycloaddition / Cleavage reactions / Sigmatropic rearrangement

Specifically Labelled Acrylamides

J. Eriksson, O. Åberg, B. Långström* 455–461

Synthesis of [\frac{11}{C}]/[\frac{13}{C}]Acrylamides by Pal-

ladium-Mediated Carbonylation

Keywords: Carbonylation / Amides Carbon monoxide / Isotopic labelling

$$R^{\times \times X} + \underbrace{\begin{array}{c} (^{13}\text{C})\text{O} \\ \text{and/or} \\ \text{[$^{11}\text{C}]\text{O}} \end{array}}_{\text{R"}} + \underbrace{\begin{array}{c} \text{Pd}_2(\text{dba})_3, \text{PPh}_3 \\ \text{THF} \end{array}}_{\text{THF}} + \underbrace{\begin{array}{c} \text{O} \\ \text{II} \\ \text{R"} \end{array}}_{\text{R"}} + \underbrace{\begin{array}{c} \text{O} \\$$

Methods for synthesizing acrylamides labelled with 11 C (β^+ , $t_{1/2} = 20.4$ min) and 13 C in the carbonyl position are presented. Labelled acrylamides were obtained in high

radiochemical yields and with high specific radioactivity by palladium-mediated carbonylative cross-coupling of vinyl halides and amines using [11C]carbon monoxide.

Chiral Tetrahydro-3-benzazepines

Asymmetric Synthesis of 1-Substituted Tetrahydro-3-benzazepines as NMDA Receptor Antagonists

Keywords: Asymmetric synthesis / Chiral auxiliary / Medicinal chemistry / 3-Benzazepines / NMDA Receptor antagonists / σ Receptor ligands / Structure affinity relationships

A novel asymmetric synthesis of enantiomerically pure tetrahydro-3-benzazepines with various substituents in position 1 is presented. Considerable enantioselective interaction with NMDA and σ receptors is observed in this substance class.

Diastereoselective Reduction

Diastereoselective Reduction of Bicyclic β -Enamino Carbonyl Piperidines — Application to the Total Synthesis of (—)-Deoxocassine.

Keywords: Reduction / Diastereoselectivity / Nitrogen heterocycles / (–)-Deoxocassine

$$R^1$$
 = H, Me R^2 = OMe, Me R^2 = Me R^2 (-)-Deoxocassine

The chemo- and diastereoselective reduction of chiral piperidine β -enamino esters and β -enamino ketones was studied and found to afford 2,3- or 2,3,6-substituted piperidines. This approach was successfully applied to the total synthesis of (–)-deoxocassine.



Novel carbocations were generated and substituted (nitrated and brominated) derivatives were synthesized from several A-ring substituted phenanthrenes. NMR, X-ray analysis and a comparative DNA binding study are reported.

A-Ring Substituted Phenanthrenium Ions

C. Brulé, K. K. Laali,* T. Okazaki, T. Musafia, W. M. Baird 487–497

Stable Ion and Electrophilic Substitution (Nitration and Bromination) Study of A-Ring Substituted Phenanthrenes: Novel Carbocations and Substituted Derivatives; NMR, X-ray Analysis, and Comparative DNA Binding

Keywords: Persistent carbocations / NMR spectroscopy / Nitration and bromination / X-ray analysis / Comparative DNA binding study

A simple and convenient preparative method for 1-aryl-2-chloro-1-ethoxyethenes is described.

Prodrug for Alzheimer's Disease

Novel Building Blocks: 1-Aryl-2-chloro-1ethoxyethenes — Preparations and Transformations

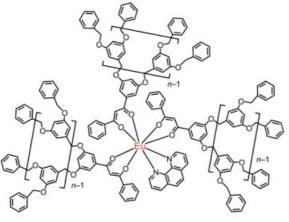
Keywords: Thiophenes / Sulfur heterocycles / Alkenes / Aryllithiums / Alzheimer's disease

Europium(III)-Core Dendrimers

B.-L. Li, Z.-T. Liu, G.-J. Deng, Q.-H. Fan* 508-516

The Synthesis of Dendritic β -Diketonato Ligands and Their Europium Complexes

Keywords: β-Diketonato ligands / Dendrimers / Europium / Luminescence



 $Eu(1-G_ndbm)_3(phen) (n = 1-3)$

Two kinds of dendritic β -diketonato ligands which contain a dibenzoylmethane (dbm) core and poly(aryl ether) dendron,

have been synthesized by a convergent strategy, and applied to the synthesis of dendritic europium(III)-core complexes.

Diastereoselective [4+2] Cycloadditions

G. Abbiati, V. Canevari, D. Facoetti, E. Rossi* 517-525

Diels-Alder Reactions of 2-Vinylindoles with Open-Chain C=C Dienophiles

Keywords: 2-Vinylindoles / Alkenes / Cycloaddition / Nitrogen heterocycles / Tetrahydrocarbazoles

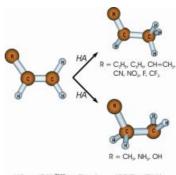
The [4+2] cycloaddition reactions between [(E)-2-vinyl]-indole-1-carboxylic acid ethyl esters and open-chain C=C dienophiles proceed with high regioselectivity giving rise to diastereoisomeric 3,4-disubstituted-1.2.3.4-tetrahydrocarbazoles.

Where Does the H⁻ Go?

R. Vianello, N. Peran. Z. B. Maksić* 526-539

Hydride Affinities of Substituted Alkenes: Their Prediction by Density Functional Calculations and Rationalisation by Triadic Formula

Keywords: Hydride affinity / Nucleophilic addition / Electron affinity / Substituent effects / Electrophilic propensity



 $HA = (EA)_n^{(Eoop} + E(\Theta a)_{nat} + (BDE) - IE(H)$

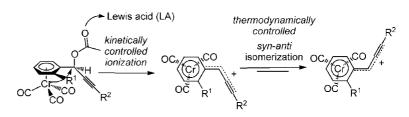
Triadic analysis provides simple rationalization and a better insight into the substituent effects on the hydride affinity of ethenes. The applied B3LYP/6-311+G(2df,p)// B3LYP/6-31G(d) level of theory proved useful and very accurate in reproducing experimentally determined hydride affinities.

Planar Chiral Cations

A. Netz, M. Drees, T. Strassner,* T. J. J. Müller* 540-547

Planar Chiral (Arene)chromiumcarbonyl-Substituted Propargyl Cations - A Spectroscopic and Computational Study

Keywords: Alkynes / Arene complexes / DFT calculations / Cations / Chromium / Spectroscopy



Characterization by UV/vis, 13C NMR, and DFT calculations

The s-syn isomers of planar chiral (arene)Cr(CO)3-substituted propargyl cations are structurally characterized by UV/Vis and 13C NMR spectroscopy. Structure, intramolecular $C_{ipso}-C_{\alpha}$ bond rotations and substituent effects are rationalized by DFT computations.

Potential Receptor Ligands

J. A. González-Vera, M. T. García-López, R. Herranz* 548-554

Regioselective Base-Promoted Nucleophilic Ring Opening of Spirocyclic Dioxopiperazines: Synthesis of N-(1-Carboxycyclohexyl)amino Acid Derivatives

Keywords: Amino acids / Spiro compounds / Imides / Piperazines / Nucleophilic addition



2,6-Dioxopiperazine-3-spirocyclohexanes are easily and regioselectively opened by hydroxide or H₂O to give N-(1-carbamoyleyclohexyl)amino acid derivatives.

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