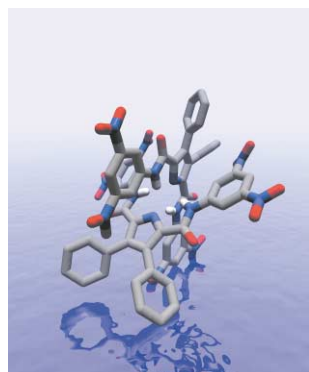


Organic & Biomolecular Chemistry

FORMERLY PERKIN TRANSACTIONS 1 AND 2

Incorporating Acta Chemica Scandinavica

**Cover**See Philip A. Gale *et al.*, page 741

The cover picture shows the crystal structure of interlocked pyrrole 2,5-diamides anions. Electron withdrawing nitro-aromatic groups have increased the acidity of the pyrrole NH proton such that addition of fluoride causes deprotonation of the pyrrole and the formation of the interlocked dimer in the solid state. In acetonitrile solution the fluoride triggered deprotonation process is accompanied by a colourless to blue colour change.

Picture by Christopher J. Woods



Chemical biology articles published in this journal also appear in the *Chemical Biology Virtual Journal*: www.rsc.org/chembiol

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Profile: *Organic & Biomolecular Chemistry* profiles Professor Varinder Aggarwal



PERSPECTIVE

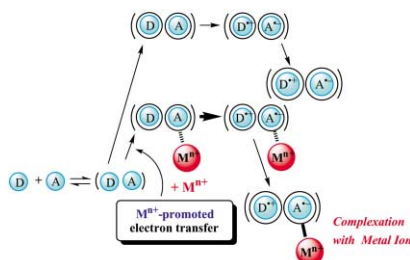
609

620

New perspective of electron transfer chemistry

Shunichi Fukuzumi

The promoting effects of metal ions (M^{n+}) on electron transfer provide a new perspective of electron transfer chemistry.

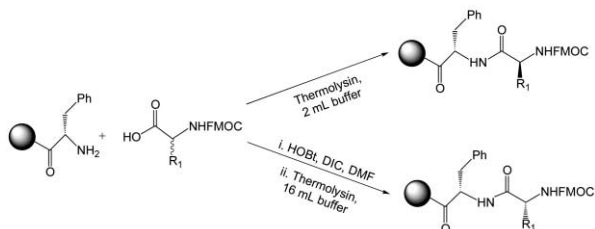


621 622

Enzymatic optical resolution *via* acylation–hydrolysis on a solid support

Rein V. Ulijn, Nicola Bisek and Sabine L. Flitsch

By taking advantage of the reversibility of the thermolysin-catalysed amide synthesis–hydrolysis reaction on a solid support, both L,L and L,D diastereoisomers of dipeptides and L-amino acids are accessible in good yields starting from enantiomeric mixtures of amino acids.



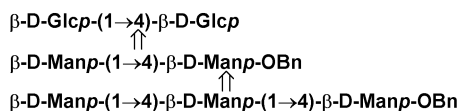
ARTICLES

623 628

The chemical synthesis of β -(1 \rightarrow 4)-linked D-mannobiose and D-mannotriose

Gavin W. J. Twaddle, Dmitry V. Yashunsky and Andrei V. Nikolaev

D-Mannobiose, prepared from D-cellobiose *via simultaneous epimerization* at C-2 and C-2', produced D-mannotriose on consecutive β -D-glucosylation and epimerization at C-2'.

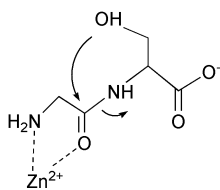


629 632

Metal-ion-assisted hydrolysis of dipeptides involving a serine residue in a neutral aqueous solution

Morio Yashiro, Yoko Sonobe, Ai Yamamura, Tohru Takarada, Makoto Komiyama and Yuki Fujii

The hydrolysis of dipeptides having a serine residue at the C-terminus, X-Ser, was remarkably promoted by $ZnCl_2$ at pH 7.0.

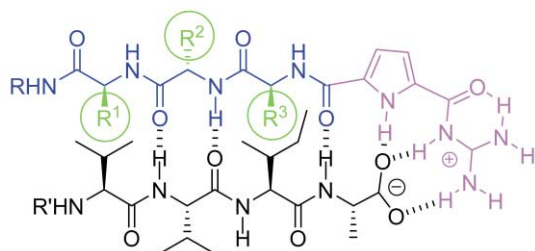


633 636

Using combinatorial methods to arrive at a quantitative structure–stability relationship for a new class of one-armed cationic peptide receptors targeting the C-terminus of the amyloid β -peptide

Carsten Schmuck and Martin Heil

Hydrophobic (green) and electrostatic interactions (blue + purple) determine the binding of tetrapeptides to a new class of one-armed cationic receptors.

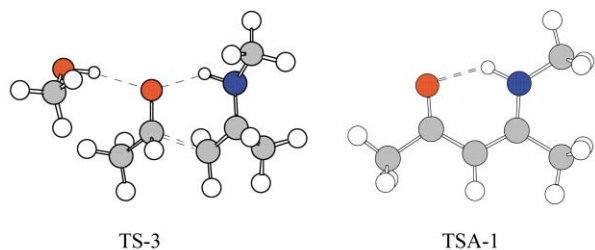


637 643

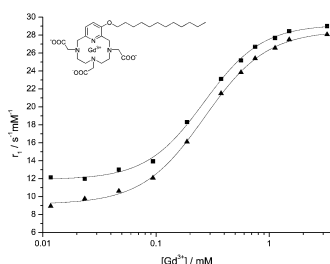
Theozyme for antibody aldolases. Characterization of the transition-state analogue

Manuel Arnó and Luis R. Domingo

Formation of two hydrogen-bonds at TS-3 favors C–C bond-formation by antibody aldolases. The transition-state analogue (TSA-1) is characterized.



644 647

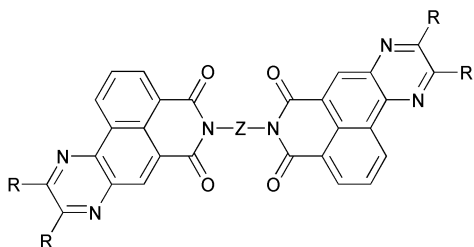


Preparation and *in vitro* evaluation of a novel amphiphilic GdPCTA-[12] derivative; a micellar MRI contrast agent

Ragnar Hovland, Christian Gløgård, Arne J. Aasen and Jo Klaveness

A novel amphiphilic GdPCTA-[12] derivative, able to form micelles with improved T_1 -relaxivity in aqueous solution, has been prepared.

648 654

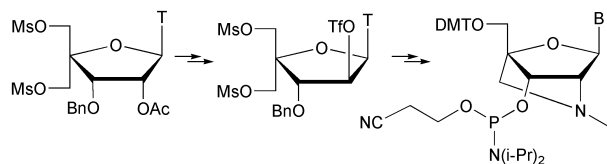


Synthesis, biological evaluation and DNA binding properties of novel mono and bisnaphthalimides

Miguel F. Braña, Mónica Cacho, Ana Ramos, M. Teresa Domínguez, Jose M. Pozuelo, Cristina Abradelo, M. Fernanda Rey-Stolle, Mercedes Yuste, Carolina Carrasco and Christian Bailly

The synthesis of a new series of potent antitumor mono and bispyrazinonaphthalimides ($IC_{50} = 17$ nM for R = H and Z = $(CH_2)_2NH(CH_2)_3NH(CH_2)_2$) is reported.

655 663



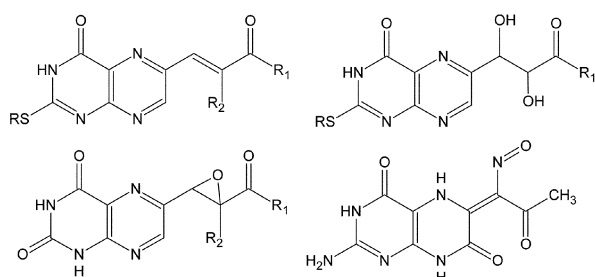
B = thymine-1-yl or 4-*N*-benzoyl-5-methyl-cytosine-1-yl

Synthesis of 2'-amino-LNA: a new strategy

Christoph Rosenbohm, Signe M. Christensen, Mads D. Sørensen, Daniel Sejer Pedersen, Lotte-Emilie Larsen, Jesper Wengel and Troels Koch

An improved route to 2'-amino-LNA that converges the syntheses of 2'-oxy-LNA and LNA analogues.

664 675

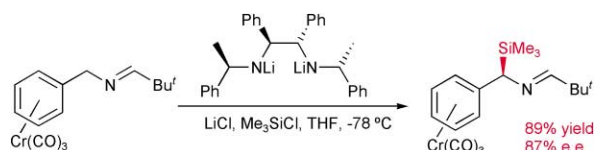


Syntheses of highly functionalised 6-substituted pteridines

Donie Guiney, Colin L. Gibson and Colin J. Suckling

Methods for the synthesis of polyfunctional 6-substituted pteridines from the corresponding 6-aldehydes are described.

676 683

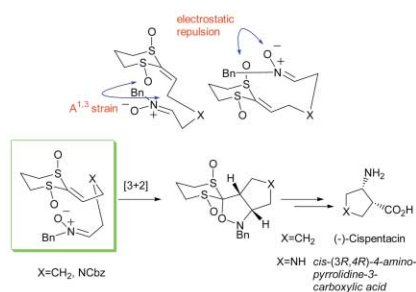


Chiral base-mediated benzylic functionalisation of tricarbonylchromium(0) complexes of benzylamine derivatives

Susan E. Gibson and Mark H. Smith

Asymmetric functionalisation of imine derivatives of the tricarbonylchromium complex of benzylamine has been achieved using a non-racemic chiral base.

684 691

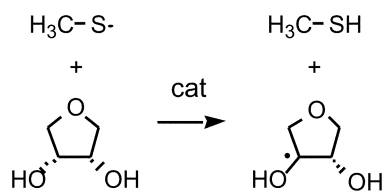


The use of enantiomerically pure ketene dithioacetal bis(sulfoxides) in highly diastereoselective intramolecular nitrene cycloadditions. Application in the total synthesis of the β -amino acid (-)-cis-pentacin and the first asymmetric synthesis of *cis*-(3*R*,4*R*)-4-amino-pyrrolidine-3-carboxylic acid

Varinder K. Aggarwal, Stephen Roseblade and Rikki Alexander

Complete diastereoselectivity was observed in the intramolecular [3+2] cycloaddition, providing an efficient route to β -amino acids.

692 699

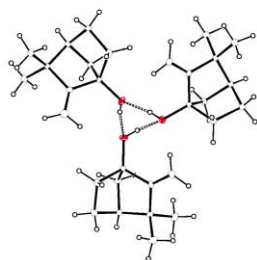


The influence of hydrogen bonding interactions on the C–H bond activation step in class I ribonucleotide reductases

Hendrik Zipse

The presence of neutral or anionic functional groups leads to a reduction of the barriers for hydrogen atom abstraction.

700 704

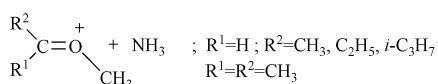


Self-recognition and hydrogen bonding by polycyclic bridgehead monoalcohols

Amelia García Fraile, David G. Morris, Antonio García Martínez, Santiago de la Moya Cerero, Kenneth W. Muir, Karl S. Ryder and Enrique Teso Vilar

Bridgehead monoalcohols hydrogen bond to form tetrameric rings and chains with pseudo-3₁ symmetry.

705 713

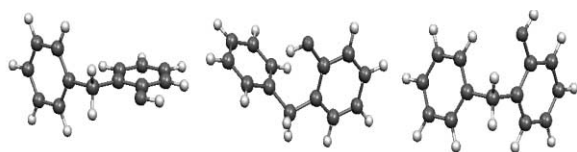


Trends in alkyl substituent effects on nucleophilic reactions of carbonyl compounds: Gas phase reactions between ammonia and R¹R²COCH₃⁺ oxonium ions

Lihn Bache-Andreassen and Einar Uggerud

The trends in reactivity are consistent with the alkyl group's electronic properties.

714 719



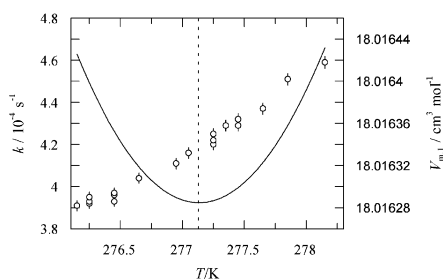
Vibrational spectra and conformational isomerism of calixarene building blocks: 2-benzylphenol

Sergei Katsyuba, Alla Chernova and Reinhard Schmutzler

The vibrational wavenumbers of the methylene bridge in bisphenylmethanes are determined by the orientation of the rings relative to the bridge plane.

$\nu_{\text{as}}\text{CH}_2$	2918 cm ⁻¹	2904 cm ⁻¹	2950 cm ⁻¹
$\nu_{\text{s}}\text{CH}_2$	2857 cm ⁻¹	2842 cm ⁻¹	2883 cm ⁻¹

720 723

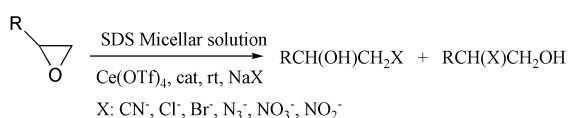


Kinetics of hydrolysis of 1-benzoyl-1,2,4-triazole in aqueous solution as a function of temperature near the temperature of maximum density, and the isochoric controversy

Michael J. Blandamer, Niklaas J. Buurma,
Jan B. F. N. Engberts and João C. R. Reis

At isochoric temperatures around the temperature of maximum density of water (TMD), rate constants for the spontaneous hydrolysis of 1-benzoyl-1,2,4-triazole at ambient pressure show no significant features which might be associated with the isochoric condition.

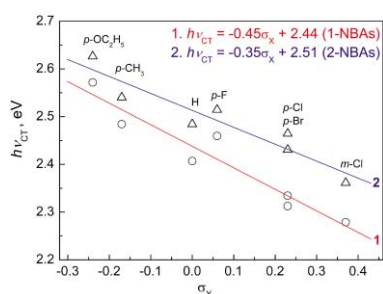
724 727



Micellar media for the efficient ring opening of epoxides with CN⁻, N₃⁻, NO₃⁻, NO₂⁻, SCN⁻, Cl⁻ and Br⁻ catalyzed with Ce(OTf)₄

Nasser Iranpoor, Habib Firouzabadi and Marzieh Shekarize
SDS micellar media was used for the ring opening reaction of epoxides with different nucleophiles at room temperature.

728 732

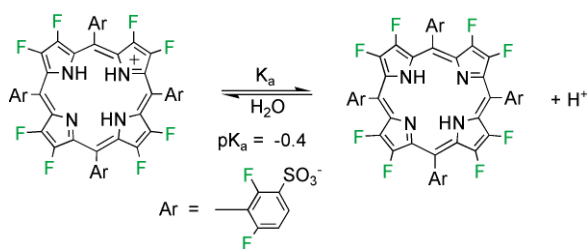


Intramolecular charge transfer with *N*-benzoylamino-naphthalenes. 1-Aminonaphthalene versus 2-aminonaphthalene as electron donors

Xuan Zhang, Chun-Hua Liu, Li-Hong Liu, Fang-Ying Wu,
Lin Guo, Xiang-Ying Sun, Chao-Jie Wang and Yun-Bao Jiang

Intramolecular charge transfer fluorescence of *N*-(substituted-benzoyl)-1-aminonaphthalenes (1-NBAs) and *N*-(substituted-benzoyl)-2-aminonaphthalenes (2-NBAs) in cyclohexane was found to show different substituent effects.

733 736

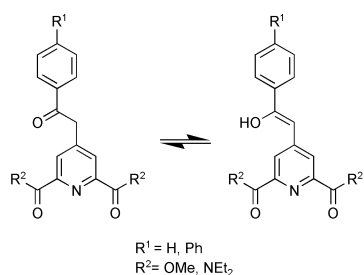


Differential substituent effects of β -halogens in water-soluble porphyrins

Justin C. Biffinger, Haoran Sun, Andrew P. Nelson and
Stephen G. DiMagno

The first water-soluble β -octafluorinated porphyrins have been prepared and their aqueous aggregation, acid–base, and optical properties have been characterized.

737 740

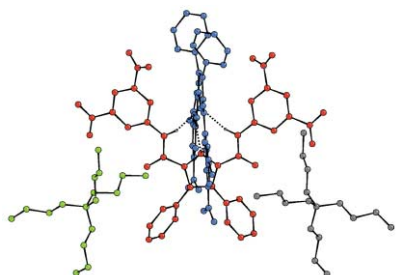


Tuning the keto equilibrium in 4-substituted dipicolinic acid derivatives

Anne-Sophie Chauvin, Sandrine Gras and
Jean-Claude G. Bünzli

The synthesis of 4-substituted dipicolinic acid derivatives requiring palladium catalysis is described. A keto–enolic equilibrium has been observed, depending on the nature of the R² substituent.

741 744

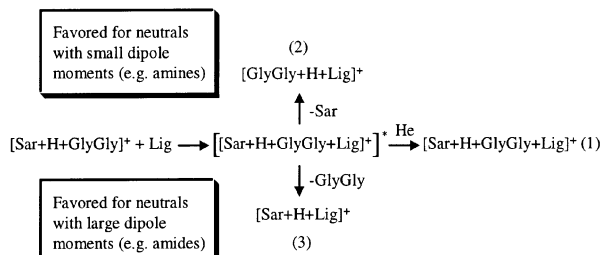


Nitrophenyl derivatives of pyrrole 2,5-diamides: structural behaviour, anion binding and colour change signalled deprotonation

Salvatore Camiolo, Philip A. Gale, Michael B. Hursthouse and Mark E. Light

An *N,N'*-bis(3,5-dinitrophenyl)-3,4-diphenyl-1*H*-pyrrole 2,5-diamide shows strong carboxylate binding in solution but is deprotonated by fluoride resulting in a colourless to blue colour change.

745 750

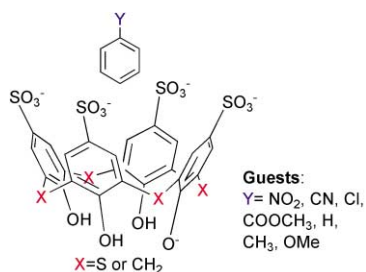


Molecular recognition in the gas phase ligand switching reactions of the proton bound dimer of sarcosine and glycylglycine

Richard A. J. O'Hair and Ana K. Vrkic

The reactions of the proton bound dimer of sarcosine and glycylglycine are probed using mass spectrometry and molecular modeling.

751 755

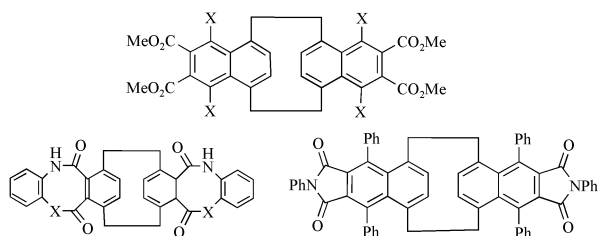


Inclusion behavior of water-soluble thiacalix- and calix[4]arenes towards substituted benzenes in aqueous solution

Noriyoshi Kon, Nobuhiko Iki and Sotaro Miyano

Thiacalix[4]arene showed higher inclusion ability than calix[4]arene suggesting that size is a more important factor in determining inclusion ability than the electron density of the calix framework.

756 761



Syntheses of various symmetrical naphthalenophanes and anthracenophanes via a Diels–Alder reaction between *syn*-[2.2](5,8)phthalazinophane derivatives and some selected dienophiles as well as the synthesis of other symmetrical heterophanes

Ashraf A. Aly

The syntheses of various classes of unreported naphthalenophanes, anthracenophanes and heterophanes are reported.



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