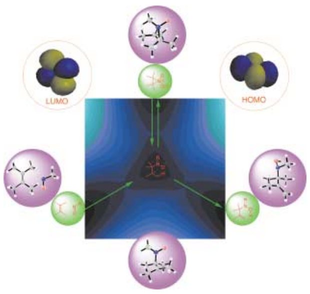
ISSN 1477-0520 OBCRAK(8) 1251–1442(2003)

Organic & Biomolecular Chemistry

FORMERLY PERKIN TRANSACTIONS 1 AND 2

Incorporating Acta Chemica Scandinavica



Cover
See A. G. Leach and K. N. Houk, page 1389. The cover picture represents the surprising potential energy surface computed for the ene reaction of nitroso compounds. The polarized diradical in the centre is a compulsory intermediate for the reaction and gives access to both the ene product and an aziridine *N*-oxide. The aziridine *N*-oxide cannot form the ene product without first reopening to the polarized diradical. Frontier molecular orbitals play a key part in dictating this mechanism. The LUMO is the antibonding π orbital but the HOMO is not the corresponding π bond but an antibonding combination of lone pairs in a plane orthogonal to the π orbital.

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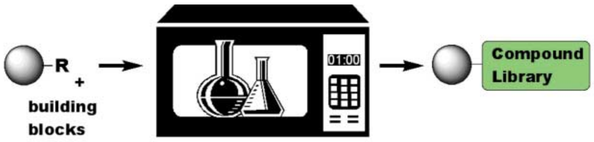
contents

EMERGING AREA

1251 1255



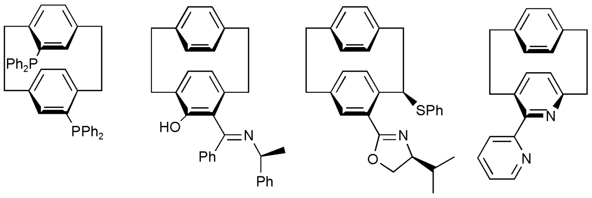
Out of the oil bath and into the oven—microwave-assisted combinatorial chemistry heats up

Helen E. Blackwell

Microwave-assisted solid-phase organic synthesis is emerging as a breakthrough technology to expedite combinatorial chemistry.

PERSPECTIVE

1256 1269



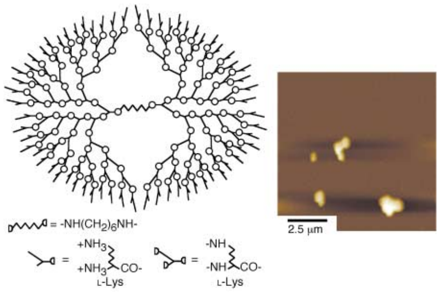
[2.2]Paracyclophane derivatives in asymmetric catalysis

Susan E. Gibson and Jamie D. Knight

A review of the use of [2.2]paracyclophanes as ligands in asymmetric catalysis is presented supplemented by a discussion of the key synthetic routes currently used to access chiral cyclophanes.

COMMUNICATIONS

1270 1273



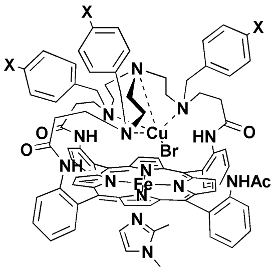
Time-dependent complex formation of dendritic poly(L-lysine) with plasmid DNA and correlation with *in vitro* transfection efficiencies

Tatsuya Okuda, Satoru Kidoaki, Mio Ohsaki, Yoshiyuki Koyama, Kenichi Yoshikawa, Takuro Niidome and Haruhiko Aoyagi

Structure of dendritic poly(L-lysine) of the 6th generation and AFM image of the complex with plasmid DNA.

1274 1276

1: X= H
2: X= N(Me)$_2$
3: X= NO$_2$



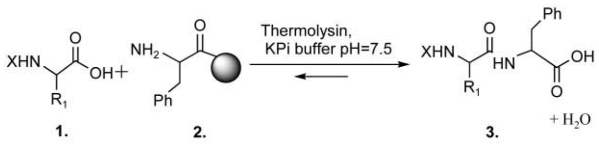
Substituted tren-capped porphyrins: probing the influence of copper in synthetic models of cytochrome *c* oxidase

Amandine Didier, Maurice L'Her and Bernard Boitrel

The synthesis of a new series of porphyrins capped with a tripod bearing either electron-donating or withdrawing groups is reported. Their electrochemical behaviour towards the catalysis of oxygen reduction has been studied.

ARTICLES

1277 1281

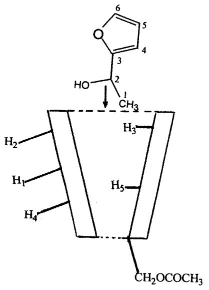


Understanding protease catalysed solid phase peptide synthesis

Rein V. Ulijn, Nicola Bisek, Peter J. Halling and Sabine L. Flitsch

Hydrophobicity of the protected amino acid substrate **1** was found to be the major contributor to the equilibrium shift towards solid phase synthesis of dipeptide **3** in bulk aqueous solution.

1282 1291

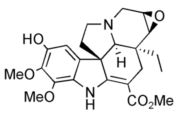


The utility of cyclodextrins in lipase-catalyzed transesterification in organic solvents: enhanced reaction rate and enantioselectivity

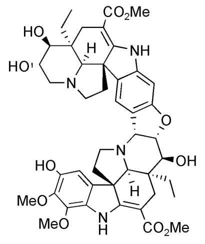
Ashraf Ghanem

The utility of cyclodextrins as additives in an enzymatic reaction is demonstrated. Evidence supporting the interaction between cyclodextrins and lipase was reported.

1292 1297



Taberhanine



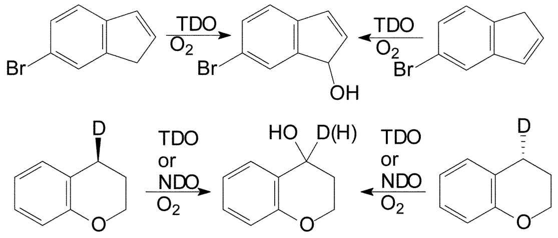
Conophyllinine

Biologically active indole and bisindole alkaloids from *Tabernaemontana divaricata*

Toh-Seok Kam, Huey-Shen Pang and Tuck-Meng Lim

The ethanol extract of the leaves of *Tabernaemontana divaricata* provided a total of 23 alkaloids including the new alkaloids taberhanine and conophyllinine.

1298 1307

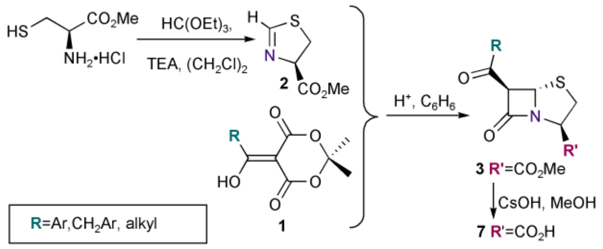


Stereochemical and mechanistic aspects of dioxygenase-catalysed benzylic hydroxylation of indene and chromane substrates

Derek R. Boyd, Narain D. Sharma, Nigel I. Bowers, Rosemary Boyle, John S. Harrison, Kyoung Lee, Timothy D. H. Bugg and David T. Gibson

Dioxygenase-catalysed benzylic hydroxylation of indene and chromane substrates is found to occur with evidence of benzylic radical involvement and mainly with retention of configuration.

1308 1314



Stereoselective synthesis of optically active bicyclic β-lactam carboxylic acids that target pilus biogenesis in pathogenic bacteria

Hans Emtenäs, Marcus Carlsson, Jerome S. Pinkner, Scott J. Hultgren and Fredrik Almqvist

β-Lactam carboxylic acids were obtained *via* rapid CsOH saponification and their chaperone binding activity was evaluated by surface plasmon resonance.

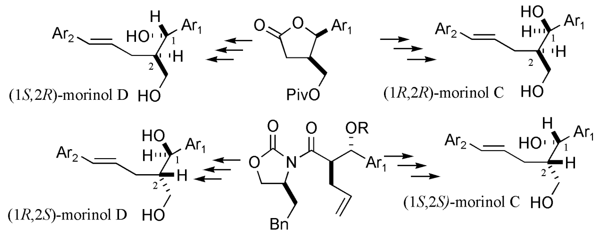
1315 1322

A proposed model of *Mycobacterium avium* complex dihydrofolate reductase and its utility for drug design

Prashant S. Kharkar and Vithal M. Kulkarni

A homology model of *Mycobacterium avium* complex dihydrofolate reductase is proposed and its utility for drug design is explained.

1323 1329



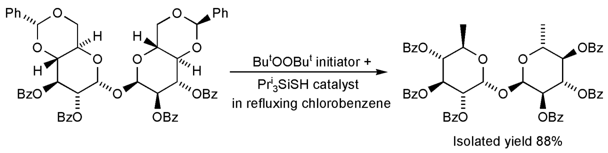
Ar_1 = 3,4-dimethoxyphenyl, Ar_2 = 4-methoxyphenyl

Syntheses of the stereoisomers of neolignans morinol C and D

Satoshi Yamauchi and Hidemitsu Uno

(1*R*,2*R*)-Morinol C and (1*S*,2*R*)-morinol D were stereoselectively synthesized from a (+)-lactone. (1*S*,2*S*)-Morinol C and (1*R*,2*S*)-morinol D were stereoselectively synthesized from the corresponding (−)-lactone prepared by an Evans' *anti*-aldol condensation. This success will contribute to the biological study of morinol C and morinol D, because the natural products are a racemic mixture.

1330 1341

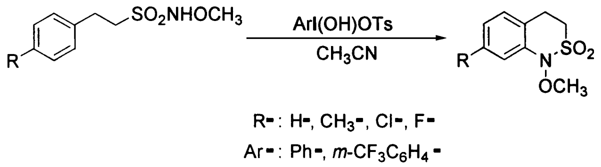


Deoxygenation of carbohydrates by thiol-catalysed radical-chain redox rearrangement of the derived benzylidene acetals

Hai-Shan Dang, Brian P. Roberts, Jasmeet Sekhon and Teika M. Smits

Carbohydrate-derived benzylidene acetals undergo an efficient thiol-catalysed radical-chain redox rearrangement to give deoxy benzoates.

1342 1346

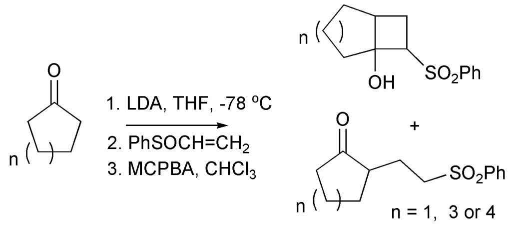


Novel preparation of 2,1-benzothiazine derivatives from sulfonamides with [hydroxy(tosyloxy)iodo]arenes

Yuhta Misu and Hideo Togo

Cyclization of sulfonamides bearing an aromatic ring at the β-position with various organohypervalent iodine compounds was carried out to form the corresponding 2,1-benzothiazine derivatives.

1347 1353

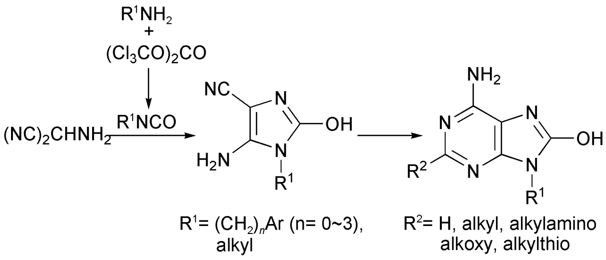


The formation of bicyclo[*n*.2.0]alkan-1-ols from the reaction of the lithium enolates of simple ketones and phenyl vinyl sulfoxide

Wendy A. Loughlin and Michelle A. McCleary

The lithium enolates of unsubstituted cyclic ketones react with phenyl vinyl sulfoxide under controlled reaction conditions to give novel bicyclo[*n*.2.0]alkan-1-ols.

1354 1365

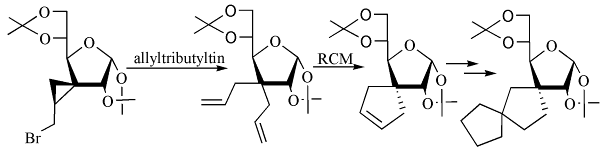


Efficient synthesis of 2,9-disubstituted 8-hydroxyadenine derivatives

Kosaku Hirota, Kazunori Kazaoka, Itaru Niimoto and Hironao Sajiki

A novel and efficient synthesis of the title compounds, which should have a range of biological activities, with various substituents is described.

1366 1373

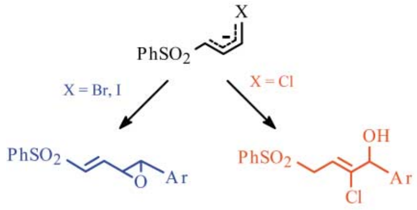


Synthesis of spirocycles *via* ring closing metathesis of heterocycles carrying *gem*-diallyl substituents obtained *via* ring opening of (halomethyl)cyclopropanes with allyltributyltin

Mukund K. Gurjar, Somu V. Ravindranadh, Kuppusamy Sankar, Sukhen Karmakar, Joseph Cherian and Mukund S. Chorghade

Simple procedure for introduction of a *gem*-diallyl group and use of RCM to prepare spirocycles.

1374 1381



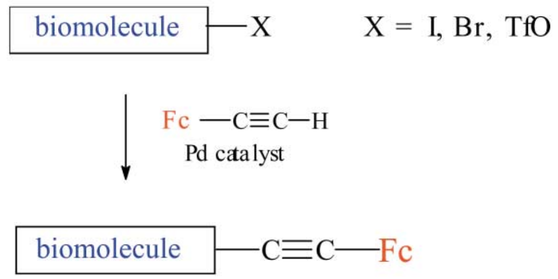
Reactions of lithiated (*E*)-3-halo-1-phenylsulfonylprop-1-enes and (*Z*)-1-halo-3-phenylsulfonylprop-1-enes with aldehydes

Eva T. Gallagher and David H. Grayson

The products formed by reactions between aryl aldehydes and the delocalised anions derived by lithiation of the title sulfones depend upon the nature of the halogen present.

ARTICLES

1382 1388

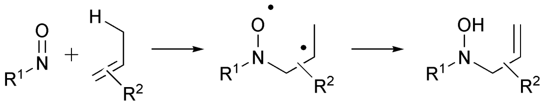


Labeling of organic biomolecules with ethynylferrocene

Evdoxia Coutouli-Argyropoulou, Maria Tsitabani,
Georgios Petrantonakis, Aris Terzis and
Catherine Raptopoulou

The attachment of ferrocene to adenine, uracil and steroid derivatives is achieved by Sonogashira coupling of ethynylferrocene.

1389 1403



The mechanism and regioselectivity of the ene reactions of nitroso compounds: a theoretical study of reactivity, regioselectivity, and kinetic isotope effects establishes a stepwise path involving polarized diradical intermediates

Andrew G. Leach and K. N. Houk

A theoretical study of the ene reactions of nitroso compounds.

1404 1408

$$A \xrightarrow{k_{1obs}} B \xrightarrow{k_{2obs}} C \xrightarrow{k_{3obs}} D$$

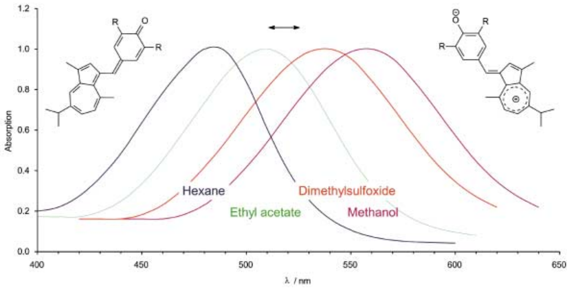
A = *N*-Methoxyphthalimide, B =*N*-Methoxyphthalamic acid
C = Phthalic anhydride, D = Phthalic acid
(i) effect of H_2O-CH_3CN on k_{1obs} at 0.001 M NaOH,
(ii) effect of H_2O-CH_3CN on k_{2obs} and k_{3obs} at 0.03 M HCl,
(iii) k_{2obs} (B) ~ k_{2obs} (phthalamic acid) ~ 10^{-1} k_{2obs} (*N*-hydroxyphthalamic acid)

Kinetics and mechanism of intramolecular carboxylic acid participation in the hydrolysis of *N*-methoxyphthalamic acid

M. Niyaz Khan and Azhar Ariffin

In order to aid the understanding of reaction mechanisms in low water content enzyme-mediated reactions, intramolecular carboxylic acid participation mechanisms in the hydrolysis of *N*-methoxyphthalamic acid have been studied.

1409 1418

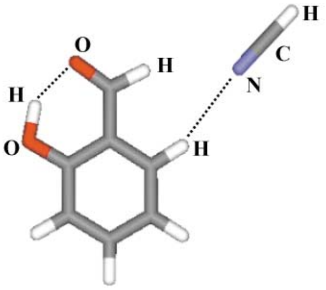


Solvatochromism, halochromism, and preferential solvation of new dipolar guaiazulenyl 1,4-benzoquinone methides

Gerhard Laus, Herwig Schottenberger, Klaus Wurst,
Johannes Schütz, Karl-Hans Ongania,
Ulrike Erika Ida Horvath and
Alexander Schwärzler

Preferential solvation of the dyes in a series of binary solvent mixtures is explained quantitatively by solvent-exchange models.

1419 1424



The effect of intramolecular interactions on hydrogen bond acidity

Farah T. T. Huque and James A. Platts

DFT calculations reveal unexpected hydrogen bonding patterns in molecules containing intramolecular hydrogen bonds.

ARTICLES

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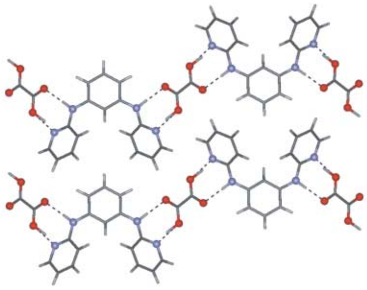
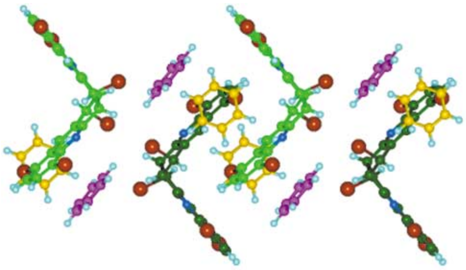


Creation of hydrogen bonded 1D networks by co-crystallization of *N*,*N′*-bis(2-pyridyl)aryldiamines with dicarboxylic acids

Igor Bensemann, Maria Gdaniec, Karina Łakomecka, Maria J. Milewska and Tadeusz Połoński

Co-crystallization of *N*,*N′*-bis(2-pyridyl)aryldiamines with dibasic acids results in formation of predictable supramolecular structures of alternating components assembled into infinite tapes.

1435 1441



Why a hexabromodiquinoline host preferentially includes small aromatic hydrocarbon guests

A. Noman M. M. Rahman, Roger Bishop, Donald C. Craig and Marcia L. Scudder

Inclusion of aromatic hydrocarbon guests by the hexabromo host **4** results in lower lattice energies by replacement of bromine–bromine interactions by aryl–aryl attractions.

CONFERENCE DIARY

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Dates, venues and contact details of forthcoming events.

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