

Organic & Biomolecular Chemistry

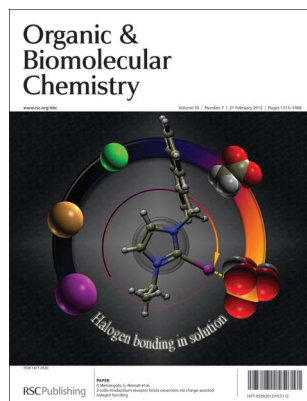
An international journal of synthetic, physical and biomolecular organic chemistry

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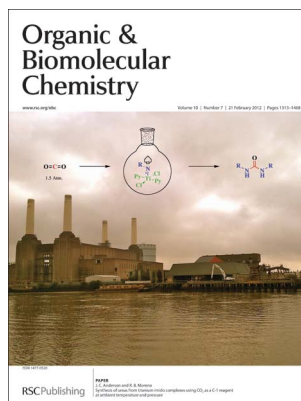
ISSN 1477-0520 CODEN OBCRAK 10(7) 1313–1468 (2012)



Cover

See P. Metrangolo, G. Resnati *et al.*, pp. 1329–1333.

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Inside cover

See J. C. Anderson and R. B. Moreno, pp. 1334–1338.

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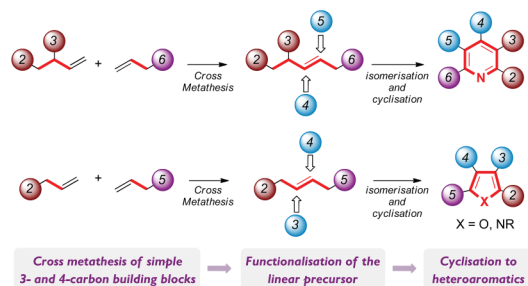
1322

Olefin cross-metathesis for the synthesis of heteroaromatic compounds

Timothy J. Donohoe,* John F. Bower and Louis K. M. Chan

The olefin cross-metathesis reaction has recently emerged as a new method for the synthesis of heteroaromatic compounds, enabling high levels of control over substitution pattern and functional group incorporation.

General CM approach to heteroaromatic compounds:



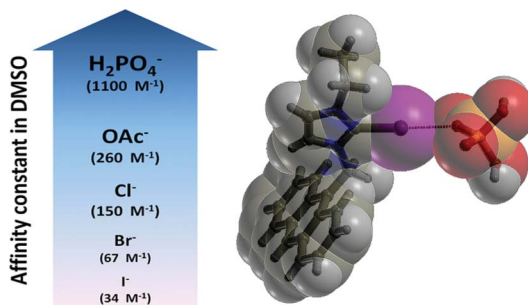
PAPERS

1329

2-Iodo-imidazolium receptor binds oxoanions *via* charge-assisted halogen bonding

Massimo Cametti, Kari Raatikainen, Pierangelo Metrangolo,* Tullio Pilati, Giancarlo Terraneo and Giuseppe Resnati*

Phosphate binds to a 2-iodo-imidazolium receptor with an association constant of *ca.* 10^3 M^{-1} , which is particularly high for a single halogen bond. A remarkably short C–I...O⁻ contact is observed in the crystal structure of the salt.



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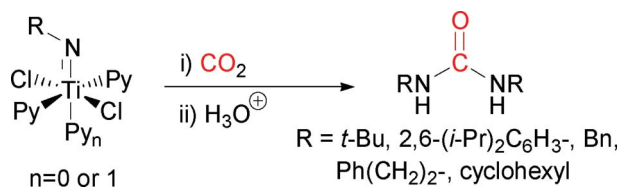
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1334

Synthesis of ureas from titanium imido complexes using CO₂ as a C-1 reagent at ambient temperature and pressure

James C. Anderson* and Rafael Bou Moreno

Certain 12- and 14- electron titanium imido complexes react with CO₂ as a C-1 reagent under ambient temperature and pressure to give ureas.

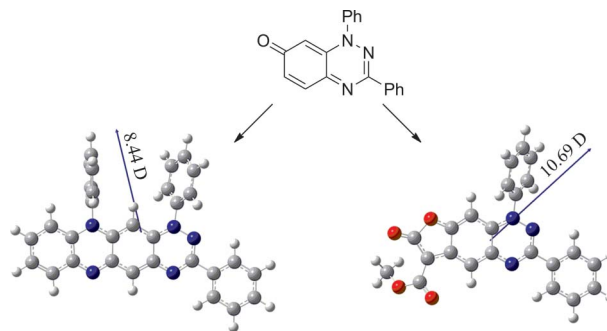


1339

Some cyclization reactions of 1,3-diphenylbenzo[e][1,2,4]-triazin-7(1H)-one: preparation and computational analysis of non symmetrical zwitterionic biscyanines

Theodosia A. Ioannou, Panayiotis A. Koutentis,* Harry Krassos, Georgia Loizou and Daniele Lo Re

1,3-Diphenylbenzo[e][1,2,4]triazin-7(1H)-one reacts with various bisnucleophiles to give a variety of deeply coloured polyazaacenes, including two zwitterionic analogues. In addition a 1,2,5-thiadiazolo fused analogue is prepared on treatment with tetrasulfur tetranitride.

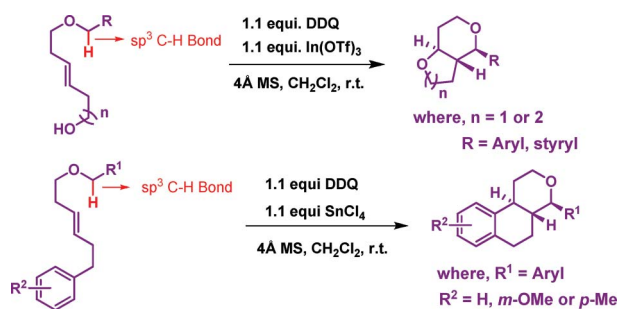


1349

Oxidative Prins and Prins/Friedel–Crafts cyclizations for the stereoselective synthesis of dioxabicycles and hexahydro-1H-benzof[iso]chromenes via the benzylic C–H activation

B. V. Subba Reddy,* Prashant Borkar, J. S. Yadav,* P. Purushotham Reddy, A. C. Kunwar, B. Sridhar and René Grée

A novel and versatile method for the stereoselective synthesis of bicyclic and tricyclic tetrahydropyran derivatives through a sequential benzylic C–H bond activation and an intramolecular Prins cyclization is described.

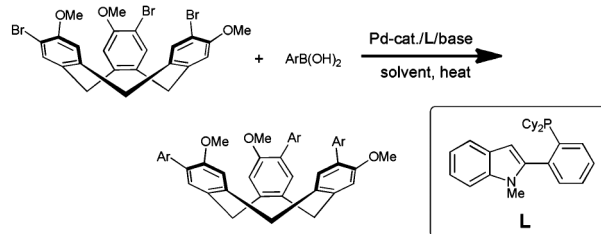


1359

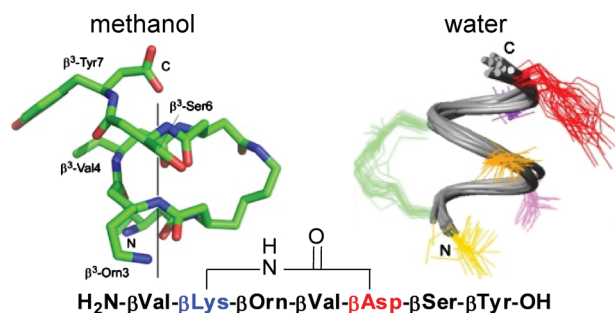
Synthesis, structure, fullerene-binding and resolution of C₃-symmetric cavitands with rigid and deep cavities

Jin-Tao Yu, Zhi-Tang Huang and Qi-Yu Zheng*

An efficient Suzuki–Miyaura coupling between CTV-Br₃ and a variety of aryl and heteroaryl boronic acids has been developed.



1365

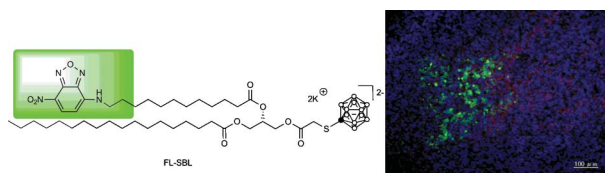


Positional screening and NMR structure determination of side-chain-to-side-chain cyclized β^3 -peptides

Esther Vaz, Sonja A. Dames, Matthias Geyer* and Luc Brunsveld*

Short β^3 -peptides fold into stable 14-helices in water *via* lactam side-chain bridging, exemplified *via* a highly compact NMR high-resolution structure.

1374

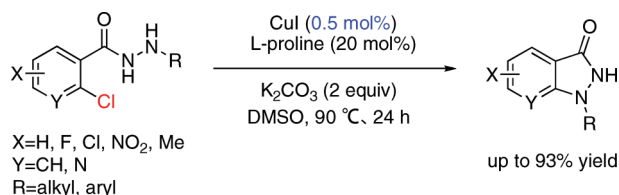


Design and synthesis of fluorescence-labeled closo-dodecaborate lipid: its liposome formation and *in vivo* imaging targeting of tumors for boron neutron capture therapy

Hiroyuki Nakamura,* Noriko Ueda, Hyun Seung Ban, Manabu Ueno and Shoji Tachikawa

We report the design and synthesis of fluorescence-labeled closo-dodecaborane lipid (FL-SBL) and its liposome formation.

1381

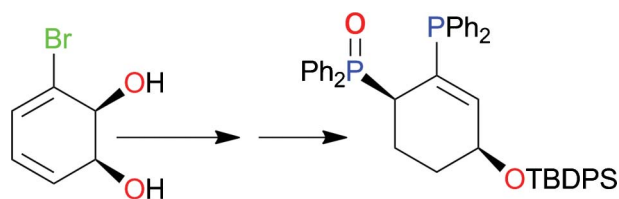


Copper-catalyzed synthesis of substituted indazoles from 2-chloroarenes at low catalyst-loading

Shinji Tanimori,* Yasuyuki Kobayashi, Yasukazu Iesaki, Yuka Ozaki and Mitsunori Kirihata

A low catalyst-loading version of indazolone synthesis based on intramolecular C–N bond formation of less reactive 2-chlorobenzhydrazide has been achieved.

1388



Chemoenzymatic synthesis of a mixed phosphine–phosphine oxide catalyst and its application to asymmetric allylation of aldehydes and hydrogenation of alkenes

Derek R. Boyd,* Mark Bell, Katherine S. Dunne, Brian Kelly, Paul J. Stevenson,* John F. Malone and Christopher C. R. Allen

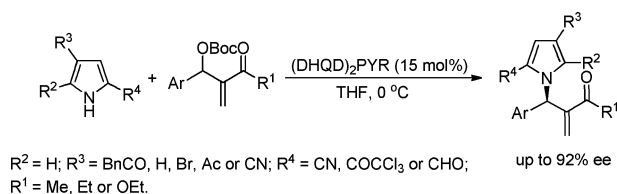
Organocatalyst for the addition of allyltrichlorosilane to aldehydes with up to 57% *ee*. Ligand for rhodium catalysed reduction of alkenes with up to 84% *ee*.

1396

Asymmetric substitutions of O-Boc-protected Morita–Baylis–Hillman adducts with pyrrole and indole derivatives

Long Huang, Yin Wei and Min Shi*

An efficient asymmetric substitution process of O-Boc-protected Morita–Baylis–Hillman adducts with various pyrrole and indole derivatives has been developed in the presence of (DHQD)₂PYR in THF, affording the corresponding products in good to high yields (up to 99%) and moderate to high ee values (up to 92 and 96%) under mild conditions.

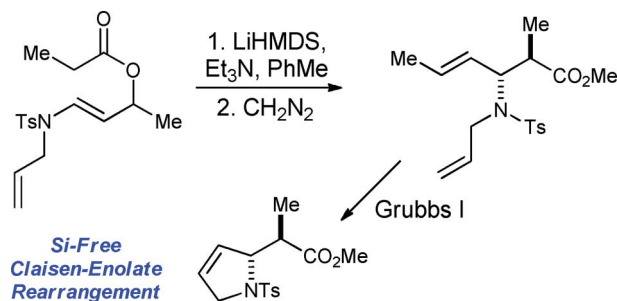


1406

Si-free enolate Claisen rearrangements of enamido substrates

Wesley R. R. Harker, Emma L. Carswell and David R. Carbery*

The Si-free Claisen enolate rearrangement of sensitive enamido-esters has been used to form α -alkyl β -amino esters with excellent stereocontrol.

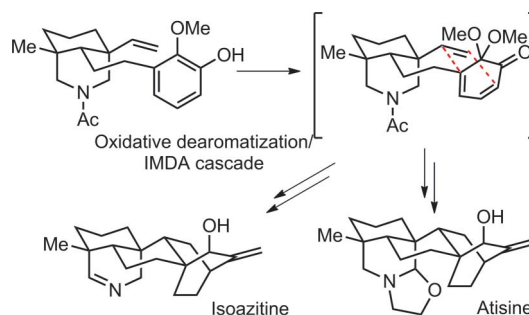


1411

Oxidative dearomatization/intramolecular Diels–Alder cycloaddition cascade for the syntheses of (±)-atisine and (±)-isoazitine

Xiao-Yu Liu, Hang Cheng, Xiao-Huan Li, Qiao-Hong Chen,* Liang Xu and Feng-Peng Wang*

A new formal synthesis of atisine and the first total synthesis of isoazitine have been accomplished.

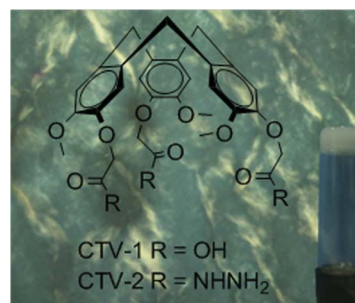


1418

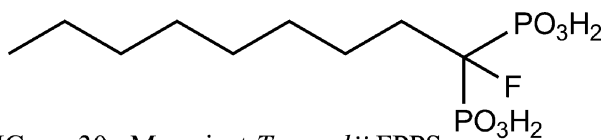
Hydrogelators of cyclotrimeratrylene derivatives

Fu Cai, Jiang-Shan Shen, Jin-He Wang, Han Zhang, Jin-Song Zhao, Er-Man Zeng* and Yun-Bao Jiang*

Rigid cavitand cyclotrimeratrylene (CTV) hydrogelators are successfully created that form luminescent optically anisotropic hydrogels with characteristic properties.



1424



IC_{50} = 30 nM against *T. gondii* FPPS

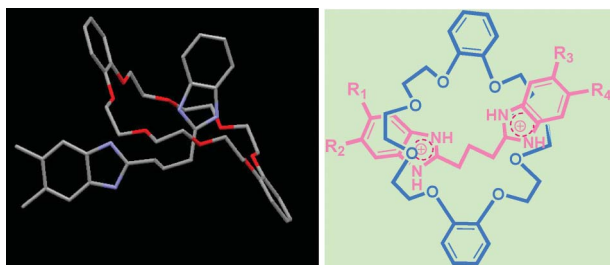
IC_{50} = 2.67 μ M against tachyzoites of *T. gondii*

1-(Fluoroalkylidene)-1,1-bisphosphonic acids are potent and selective inhibitors of the enzymatic activity of *Toxoplasma gondii* farnesyl pyrophosphate synthase

Sergio H. Szajnman, Valeria S. Rosso, Leena Malayil, Alyssa Smith, Silvia N. J. Moreno, Roberto Docampo and Juan B. Rodriguez*

α -Fluorinated-1,1-bisphosphonic acids were designed, synthesized and biologically evaluated against *Trypanosoma cruzi*, *Toxoplasma gondii* and the target parasitic enzymes farnesyl pyrophosphate synthase of *T. cruzi* and *T. gondii*.

1434

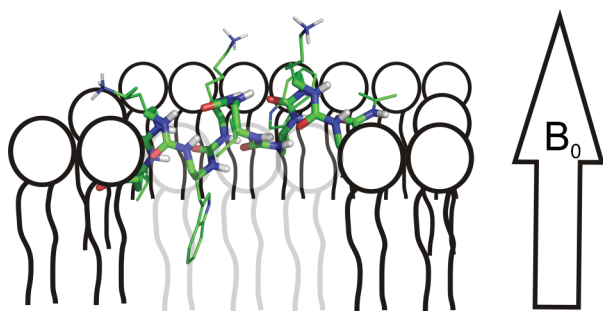


Unraveling the molecular recognition of “three methylene spacer” bis(benzimidazolium) moiety by dibenzo-24-crown-8: pseudorotaxanes under study

Chhanda Mukhopadhyay,* Sabari Ghosh and Ann Marie Schmiedekamp

“Three methylene spacer” bis(benzimidazolium) derivatives act as a new template threading dibenzo-24-crown-8 into [2]pseudorotaxanes.

1440

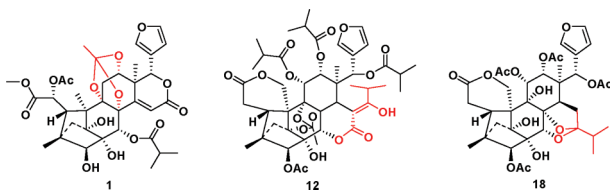


Solid state NMR studies of oligourea foldamers: Interaction of 15 N-labelled amphiphilic helices with oriented lipid membranes

Christopher Aisenbrey, Nagendar Pendem, Gilles Guichard* and Burkhard Bechinger*

The 15 N-chemical shift tensor of urea bonds is determined and the bilayer topology of an antimicrobial oligourea analysed.

1448



Kv1.2 potassium channel inhibitors from *Chukrasia tabularis*

Hong-Bing Liu, Hua Zhang, Ping Li, Yan Wu, Zhao-Bing Gao and Jian-Min Yue*

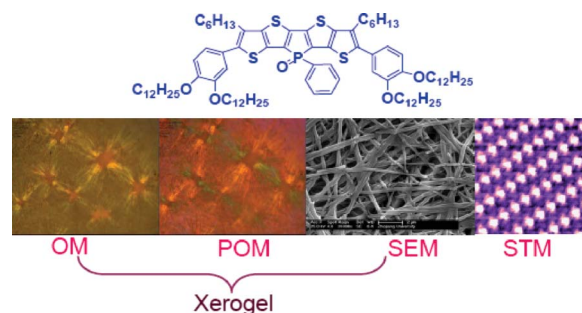
A series of limonoids, chubularisins A–R, obtained from *Chukrasia tabularis*, displayed potent and selective inhibition against the delayed rectifier (I_K) K^+ current.

1459

Phosphole modified pentathienoacene: Synthesis, electronic properties and self-assembly

Jun-Hua Wan,* Wei-Fen Fang, Yi-Bao Li, Xu-Qiong Xiao, Li-Hong Zhang, Zheng Xu, Jia-Jian Peng and Guo-Qiao Lai*

Phosphole modified pentathienoacene with a much lower LUMO level can self-assemble into different supramolecular structures with the aid of long alkyl chains.



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