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ISSN 1144–0546 CODEN NJCHES 30(3) 289–492 (2006)

Cover
See Stefano Moro *et al.*, page 301.
New perspectives on the complexity of G protein-coupled receptor (GPCR) signalling and the increased resolution of existing tools for studying GPCR behaviour has led to the conception of new hypotheses that affect the discovery of ligands (both agonists and antagonists) acting at GPCRs. Deciphering structure–function relationships in GPCRs will promote computer-aided drug discovery by elucidating the binding mode(s) of known ligands into their receptor binding-sites.
Image reproduced by permission of Stefano Moro, Magdalena Bacilieri, Francesca Deflorian and Giampiero Spalluto, *New J. Chem.*, 2006, **30**, 301.

CHEMICAL SCIENCE

C17

Drawing together the research highlights and news from all RSC publications, *Chemical Science* provides a ‘snapshot’ of the latest developments across the chemical sciences showcasing newsworthy articles, as well as the most significant scientific advances.

Chemical Science
March 2006/Volume 3/Issue 3
www.rsc.org/chemicalscience

PERSPECTIVE

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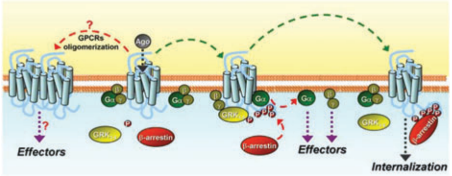
G protein-coupled receptors as challenging druggable targets: insights from *in silico* studies

Stefano Moro,* Magdalena Bacilieri, Francesca Deflorian and Giampiero Spalluto

The application of structure-based computational methods to drug discovery is still considered a major challenge, especially when the target is a G protein-coupled receptor.



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LETTERS

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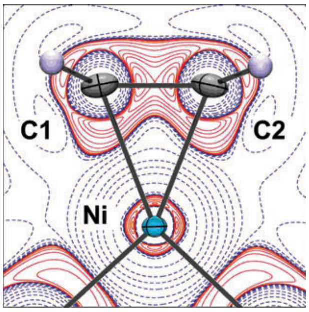
Valence shell charge concentrations and the Dewar–Chatt–Duncanson bonding model

Wolfgang Scherer,* Georg Eickerling, Dmitry S, Emanuel Gullo, G. Sean McGrady and Peter Sirsch

Combined experimental and theoretical charge density studies of the complex $[Ni(\eta^2\text{-}C_2H_4)dbpe]$ (dbpe = $Bu^t_2PCH_2CH_2PBu^t_2$) reveal how the location and magnitude of charge concentrations in the valence shell of the metal atom influence the σ- and π-components of the metal–olefin interaction.



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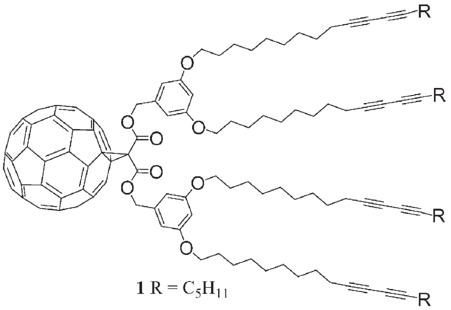
Towards polymerizable fullerene derivatives to stabilize the initially formed phases in bulk-heterojunction solar cells

Jean-François Nierengarten* and Sepas Setayesh*

Photovoltaic cells have been prepared with blends of polymerizable methanofullerene derivative **1** bearing four butadiyne subunits and MDMO-PPV; annealing at 100 °C for 2 hours resulted in an improvement of the performances of the devices.



1 $R = C_5H_{11}$

PAPERS

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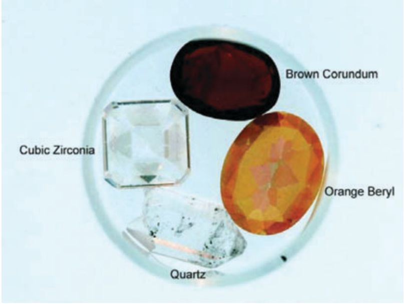
Neoteric optical media for refractive index determination of gems and minerals

Maggel Deetlefs, Kenneth R. Seddon and Michael Shara

A range of ionic liquids (many novel) based on the 1-alkyl-3-methylimidazolium cation, have been prepared and can be used as relatively benign immersion fluids for optical mineralogy studies. In addition, for a series of ionic liquids with the same anion, it is shown that the refractive indices can be adjusted by systematic changes in the cation.



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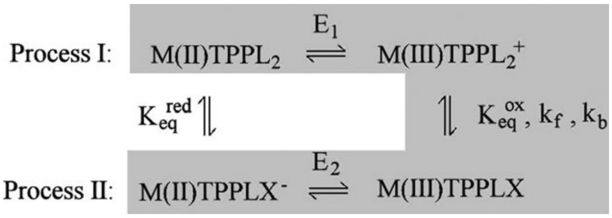
The electrochemical ion-transfer reactivity of porphyrinato metal complexes in 4-(3-phenylpropyl)pyridine | water systems

Michael J. Bonné, Christopher Reynolds, Stuart Yates, Galyna Shul, Joanna Niedziolka, Marcin Opallo and Frank Marken*

Porphyrinato metal complexes undergo oxidation/reduction processes which are coupled to anion and cation transfer processes in organic solvent | water two phase systems.



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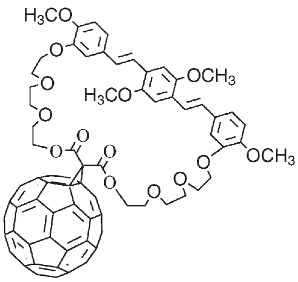

Synthesis and photoresponse of a fullerene–bis(styryl)benzene dyad

Nadia Camaioni,* Graziano Fabbrini, Enzo Menna, Michele Maggini,* Giovanni Ridolfi and Alberto Zanelli

A macrocyclic bis(styryl)benzene–fullerene dyad works as an active component in solar cells.

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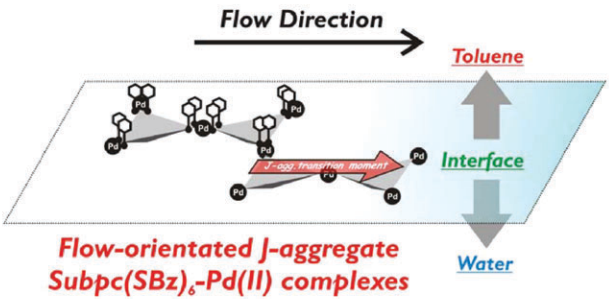

Two-phase Couette flow linear dichroism measurement of the shear-forced orientation of a palladium(II)-induced aggregate of thioether-derivatised subphthalocyanines at the toluene/glycerol interface

Kenta Adachi and Hitoshi Watarai*

An interfacial flow-oriented J-aggregate of **Subpc(SBz)$_6$**–Pd(II) complexes (illustrated), in which the transition dipole is aligned in one direction at the toluene/water interface, has been successfully prepared in a two-phase Couette flow (TPCF) system.

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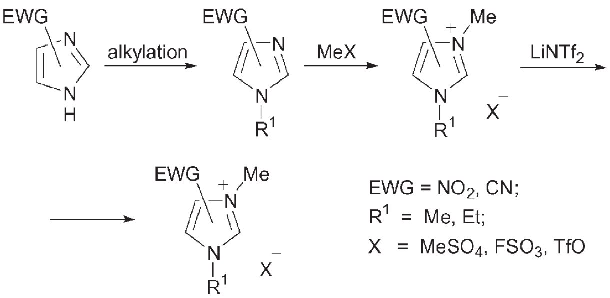

Strategies toward the design of energetic ionic liquids: nitro- and nitrile-substituted *N,N′*-dialkylimidazolium salts

Alan R. Katritzky,* Hongfang Yang, Dazhi Zhang, Kostyantyn Kirichenko, Marcin Smiglak, John D. Holbrey,* W. Matthew Reichert and Robin D. Rogers*

Twelve novel 1,3-dialkylimidazolium salts containing strongly electron-withdrawing nitro- and cyano-functionalities directly appended to the cationic heterocyclic rings have been synthesized.

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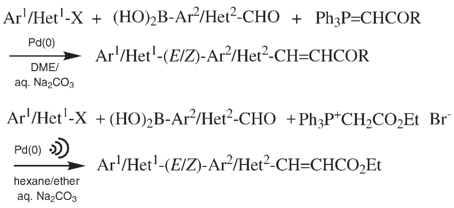

One-pot Wittig olefination–Suzuki reaction—the compatibility of conjugated phosphoranes in Pd(0) catalysed C–C-bond forming reactions

Thies Thiemann,* Masataka Watanabe, Yasuko Tanaka and Shuntaro Mataka

Suzuki cross-coupling and Wittig reactions can be combined in one step. The use of ultrasound allows the reaction to be run in a mixture of hexane–ether at low bulk temperatures.

PAPERS

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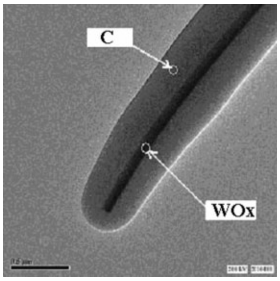
Growth of carbon sausages filled with *in situ* formed tungsten oxide nanorods: thermal dissociation of tungsten(VI) isopropoxide in isopropanol

Swati V. Pol, Vilas G. Pol, Vadim G. Kessler and Aharon Gedanken*

A simple, one-stage, efficient synthetic method for the growth of **c**arbon **s**ausages filled with *in situ* formed **t**ungsten **o**xide **n**anorods (CSTON), without any external catalyst is reported.



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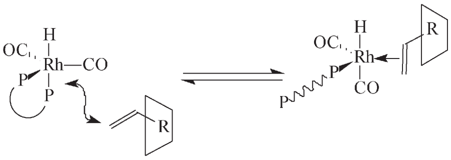
Hydroformylation of 1-decene in aqueous medium catalysed by rhodium–alkyl sulfonated diphosphines system in the presence of methylated cyclodextrins. How the flexibility of the diphosphine backbone influences the regioselectivity

Sébastien Tilloy,* Grégory Crowyn, Eric Monflier, Piet W. N. M. van Leeuwen and Joost N. H. Reek

Methylated cyclodextrins induce the formation of low-coordinated phosphine species.



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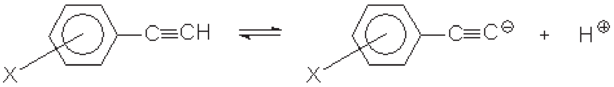
Range of validity of the Hammett equation: acidity of substituted ethynylbenzenes

Stanislav Böhm, Patrik Pařík and Otto Exner*

While the protonation of *meta*-substituted ethynylbenzenes follows the Hammett equation with high precision, *para*-derivatives show characteristic large deviations. On the basis of 16 reaction series with 295 compounds it is suggested that validity of the Hammett equation should be restricted to *meta*-derivatives in exact studies.



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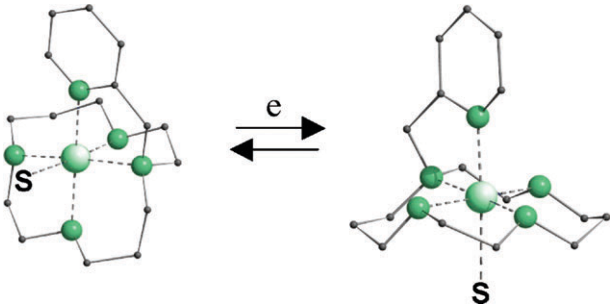
Nickel(II) complexes of cyclen- and cyclam-pyridine: topological reorganisations induced by electron transfer

Sanae El Ghachtouli, Cyril Cadiou, Isabelle Déchamps-Olivier, Françoise Chuburu,* Michel Aplincourt, Véronique Patinec, Michel Le Baccon, Henri Handel and Thierry Roisnel

Electrochemical studies on nickel(II) cyclam-pyridine complexes have underlined a redox-triggered movement between configurational isomers.



PAPERS

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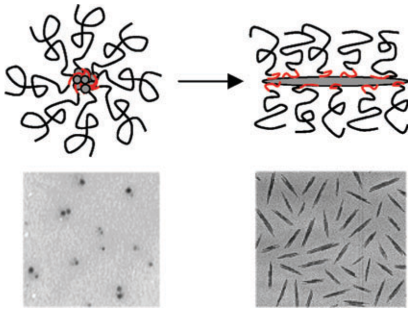

Hydrophilic block copolymer-directed growth of lanthanum hydroxide nanoparticles

Frédéric Bouyer, Nicolas Sanson, Mathias Destarac and Corine Gérardin*

The shape and size of polymer-stabilized metal hydroxide nanoparticles can be controlled by varying the characteristics of the precursor copolymer–metal ion complexes.

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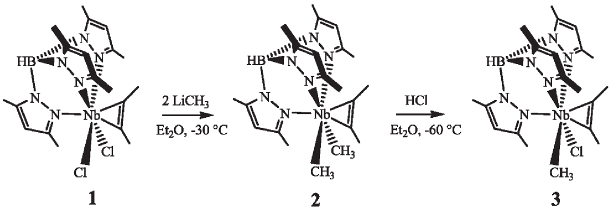

Synthesis and structural characterisation of $[\mathrm{Tp^{Me2}Nb(CH_3)_2(CH_3C{\equiv}CCH_3)}]$ and $[\mathrm{Tp^{Me2}NbCl(CH_3)(CH_3C{\equiv}CCH_3)}]$: is there an intrinsic α-agostic interaction in alkyl complexes of the $[\mathrm{Tp^{Me2}Nb(alkyne)}]$ moiety?

Emmanuelle Teuma, Michel Etienne,* Bruno Donnadieu and G. Sean McGrady*

The methyl complexes **2** and **3** have been studied by XRD, IR and NMR.

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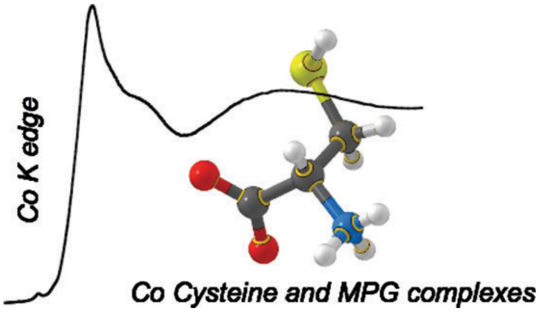

XAS Investigation of biorelevant cobalt complexes in aqueous media

C. Bresson, S. Esnouf, C. Lamouroux, P. L. Solari and C. Den Auwer*

Aqueous cobalt(II)/(III) complexes of biorelevant cysteine and *N*-2-mercaptopropionylglycine (MPG) ligands investigated by X-ray absorption spectroscopy.

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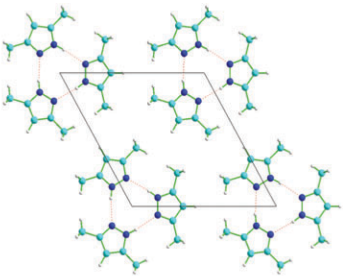

Molecular dynamics of the self-organising strong hydrogen bonded 3,5-dimethylpyrazole

John A. Stride,* Upali A. Jayasooriya, Jean-Marc Zanotti and Remi Kahn

Selective isotopic substitution in the strongly hydrogen-bonded, self-organising system 3,5-dimethylpyrazole allows for the characterisation of molecular re-orientations using quasielastic neutron scattering. The proton motion perpendicular to the hydrogen-bonds is shown to be largely independent of the methyl torsional rotations.

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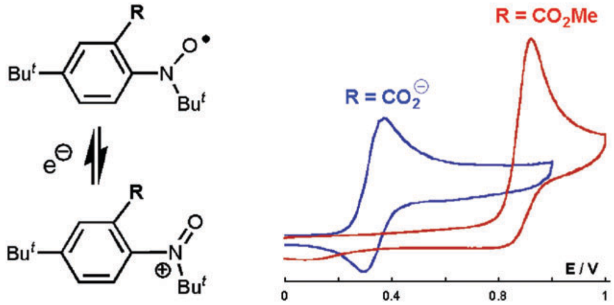
Intramolecular charge effects in the electrochemical oxidation of aminoxyl radicals

Lucien Marx and Bernd Schöllhorn*

The redox properties of aromatic nitroxides are strongly dependent on the presence of a negative charge in proximity to the aminoxyl group causing a particularly high potential shift.



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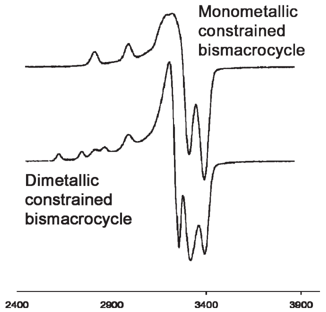
New side-bridged bismacrocycles and cross-bridged macrotricycles. Syntheses and Cu(II) complexation study

Nicolas Bernier, Mustapha Allali, Raphaël Tripier, Françoise Conan, Véronique Patinec, Stéphanie Develay, Michel Le Baccon and Henri Handel*

Constrained bismacrocyclic and macrotricyclic polyamines have been synthesized and their mono- and dimetallic copper(II) complexes characterized by electronic and EPR spectroscopy.



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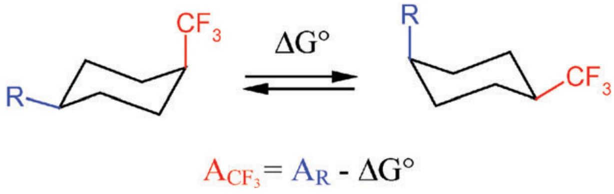
Experimental determination of the conformational free energies (*A* values) of fluorinated substituents in cyclohexane by dynamic ^{19}F NMR spectroscopy. Part 1. Description of the method for the trifluoromethyl group

Yvan Carcenac, Patrick Diter, Claude Wakselman and Marc Tordeux*

The *A* value of the trifluoromethyl group was determined by ^{19}F NMR studies, and the thermodynamic parameters (ΔG°, ΔH°, ΔS°) are given.



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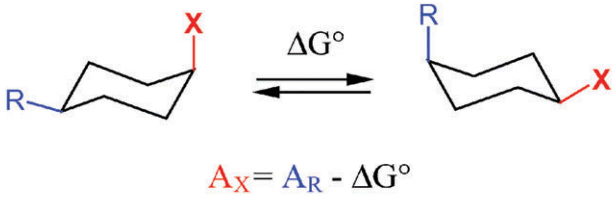
Experimental determination of the conformational free energies (*A* values) of fluorinated substituents in cyclohexane by dynamic ^{19}F NMR spectroscopy. Part 2. Extension to fluoromethyl, difluoromethyl, pentafluoroethyl, trifluoromethylthio and trifluoromethoxy groups

Yvan Carcenac, Marc Tordeux, Claude Wakselman and Patrick Diter*

The *A* values ($-\Delta G^\circ_{298K}$) of various fluoro-containing groups were obtained: 1.59 (CFH_2), 1.85 (CF_2H), 2.67 (C_2F_5), 0.79 (OCF_3) and 1.18 (SCF_3) [in kcal mol^{-1}].



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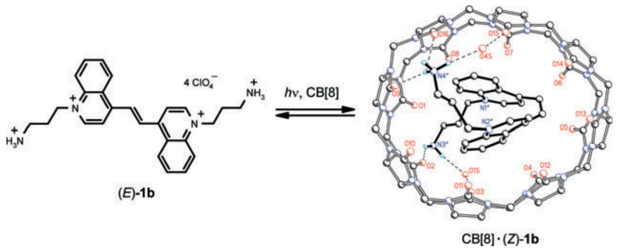

Photoinduced and dark complexation of unsaturated viologen analogues containing two ammonium tails with cucurbit[8]uril

Lyudmila G. Kuz'mina,* Artem I. Vedernikov, Natalia A. Lobova, Judith A. K. Howard, Yuri A. Strelenko, Vladimir P. Fedin, Michael V. Alfimov and Sergey P. Gromov*

Structure and stability of complexes between cucurbit[8]uril and diammonium viologen analogues were studied by NMR spectroscopy and X-ray diffraction.

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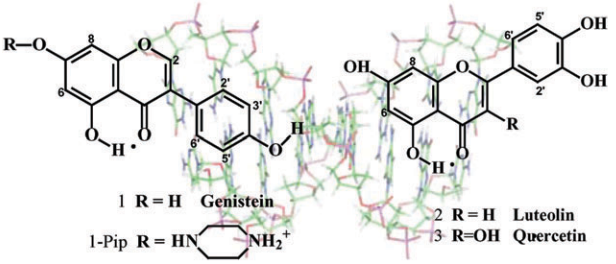

Interaction of flavonoid topoisomerase I and II inhibitors with DNA oligomers

Wojciech Bocian,* Robert Kawęcki, Elżbieta Bednarek, Jerzy Sitkowski, Agnieszka Ulkowska and Lech Kozerski*

The binding affinities of flavonoids, genistein and quercetin, to DNA oligomers have been evaluated by NMR studies and MP2 and DFT calculations used to assess the binding mode of genistein to DNA.

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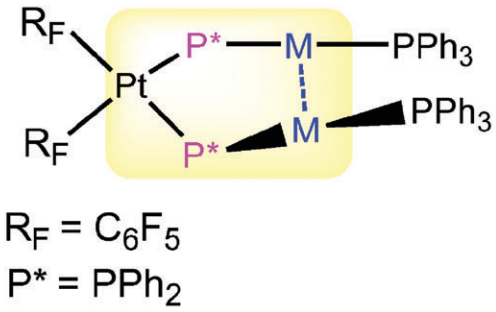

Coordination of a monomeric diphosphido platinum complex as a bridging ligand

Jesús R. Berenguer, Naima Chaouche, Juan Forniés,* Consuelo Fortuño and Antonio Martín

The heterotrinuclear complexes $[M_2Pt(\mu\text{-}PPh_2)_2(C_6F_5)_2(PPh_3)_2]$ (M = Au **1**, Ag **2**) do not display Pt–M bonds but M···M bonding interactions, which according to NMR spectra, seem to be present in solution at low temperature.

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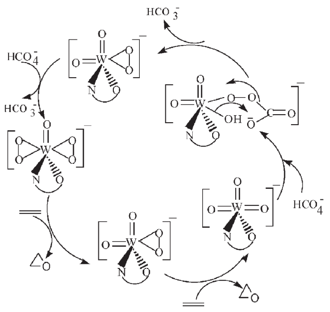

Highly facile homogeneous epoxidation of olefins using oxo-diperoxo tungstate(VI) complex as catalyst, bicarbonate as co-catalyst and hydrogen peroxide as a terminal oxidant

Swarup K. Maiti, Subhajit Dinda, Narottam Gharah and Ramgopal Bhattacharyya*

Bicarbonate activated H_2O_2 in the presence of catalytic PPh_4 $[WO(O_2)_2(QO)]$ shows unmatched efficiency in olefin epoxidation at rt. The TOF varies from 59 400 to 352 h^{-1}, depending on the substrate.

ADDITIONS AND CORRECTIONS

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Highly facile homogeneous epoxidation of olefins using oxo-diperoxo tungstate(VI) complex as catalyst, bicarbonate as co-catalyst and hydrogen peroxide as a terminal oxidant

Swarup K. Maiti, Subhajit Dinda, Narottam Gharah and Ramgopal Bhattacharyya

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