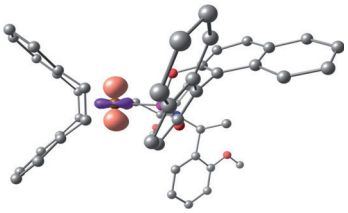
Reaction Mechanisms

J. A. Raskatov, M. Jäkel, B. F. Straub, F. Rominger, G. Helmchen*

Iridium-Catalyzed Allylic Substitutions with Cyclometalated Phosphoramidite Complexes Bearing a Dibenzocyclooctatetraene Ligand: Preparation of (π-Allyl)Ir Complexes and Computational and NMR Spectroscopic Studies

Bigger is better: The replacement of cod by dibenzo-cot is worth the effort because (allyl)Ir complexes of the latter compound are catalysts that give rise to improved regioselectivity and stability in iridium-catalyzed allylic aminations and alkylations.



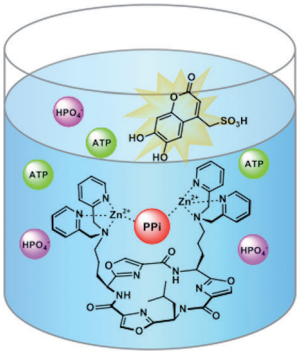
Chem. Eur. J.
DOI: **10.1002/chem.201201772**

Molecular Recognition

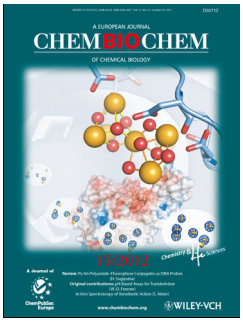
S. J. Butler, K. A. Jolliffe*

Selective Pyrophosphate Recognition by Cyclic Peptide Receptors in Physiological Saline

Mixing in different circles: Cyclic peptide-based receptors bind preferentially to pyrophosphate (PPi) over ATP, ADP, and phosphate in physiological saline (Krebs buffer). Selectivity for PPi over ATP and ADP is significantly enhanced in this biologically relevant fluid in comparison to that observed in water.



Chem. Asian J.
DOI: **10.1002/asia.201200627**

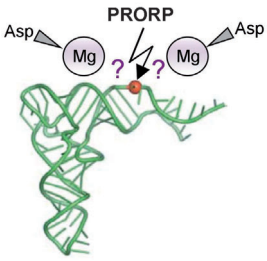


Kinetics

L. V. Pavlova, M. Gößringer, C. Weber, A. Buzet, W. Rossmanith, R. K. Hartmann *

tRNA Processing by Protein-Only versus RNA-Based RNase P: Kinetic Analysis Reveals Mechanistic Differences

Proteinaceous! *R*p-phosphorothioate modification at the RNase P cleavage site reveals that the catalytic mechanism utilized by proteinaceous RNase P (PRORP) is different from that of RNA-based bacterial RNase P, taking place without a direct metal-ion coordination to the (pro-)*R*p substituent.



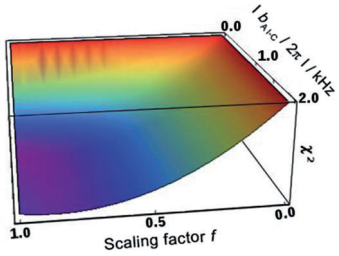
ChemBioChem
DOI: **10.1002/cbic.201200434**

Nuclear Magnetic Resonance

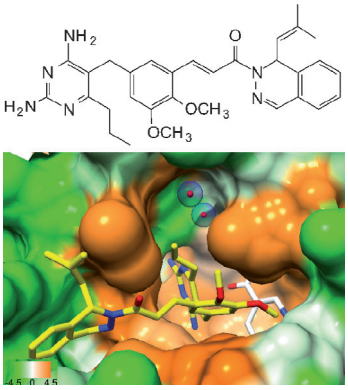
F. Pourpoint,* J. Trébosc, R. M. Gauvin, Q. Wang, O. Lafon, F. Deng, J.-P. Amoureux*

Measurement of Aluminum–Carbon Distances Using S-RESPDOR NMR Experiments

Going the distance: Aluminum–carbon internuclear distances can be measured in samples with ^{13}C natural abundance by rapid fitting of experimental NMR data to an analytical expression (e.g. for a tetraalkyl aluminate, see picture). A combination of ^{27}Al saturation pulse with heteronuclear dipolar recoupling yields dipolar dephasing of the ^{13}C signal, which only depends on the Al–C distance and the efficiency of the pulse.



ChemPhysChem
DOI: **10.1002/cphc.201200490**



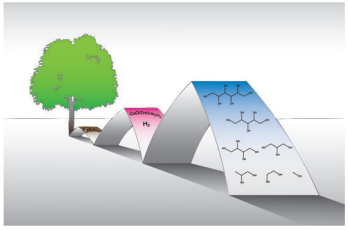
ChemMedChem
DOI: **10.1002/cmdc.201200291**

Antibiotics

B. Nammalwar, C. R. Bourne,* R. A. Bunce,* N. Wakeham, P. C. Bourne, K. Ramnarayan, S. Mylvaganam, K. D. Berlin, E. W. Barrow, W. W. Barrow

Inhibition of Bacterial Dihydrofolate Reductase by 6-Alkyl-2,4-diaminopyrimidines

From resistance to terrorism: A series of (±)-6-alkyl-2,4-diaminopyrimidines was synthesized and evaluated for inhibition of bacterial dihydrofolate reductase (DHFR). Biological studies revealed slightly attenuated activity relative to structures lacking C6 alkyl substitution. This arises from a conformational change of the protein resulting in exposure of a hydrated pocket contiguous with the existing binding site.



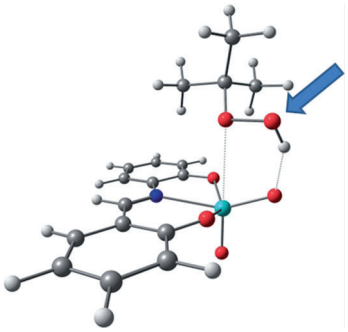
ChemSusChem
DOI: **10.1002/cssc.201200482**

Biomass Conversion

K. Tajvidi, K. Pupovac, M. Kükrek, R. Palkovits*

Copper-Based Catalysts for Efficient Valorization of Cellulose

Noble causes: Cellulose is effectively converted into methanol, propylene, and ethylene glycol over Cu-based catalysts. Overall yields of above 93%, together with 63% yield of C_1–C_3 compounds, can be reached over simple noble-metal-free systems, opening new opportunities for the sustainable and cost-efficient valorization of cellulose.



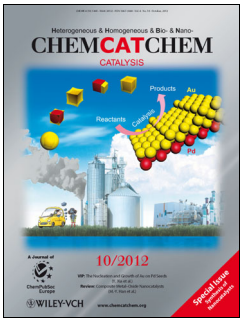
ChemCatChem
DOI: **10.1002/cctc.201200068**

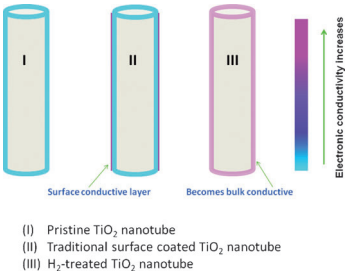
Epoxidation

J. Morlot, N. Uyttebroeck, D. Agustin,* R. Poli*

Solvent-Free Epoxidation of Olefins Catalyzed by "[MoO_2(SAP)]": A New Mode of *tert*-Butylhydroperoxide Activation

A Bartlett ballet: $[MoO_2L]_2$ complexes (L = SAP, SAE, SAMP) are active and selective precatalysts for the epoxidation of cyclooctene using *tert*-butylhydroperoxide (TBHP) in water as oxidant and no extra solvent. According to the DFT study; the TBHP oxidant coordinates 5-coordinate "[MoO_2(SAP)]" as a neutral molecule; the way in which this transfers the O atom to the external olefin is reminiscent of Bartlett's epoxidation by peroxyacids.





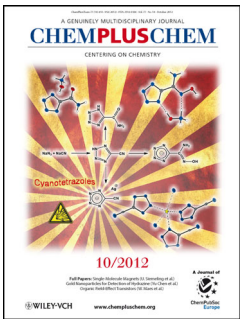
ChemPlusChem
DOI: **10.1002/cplu.201200104**

Microbatteries

Z. Lu,* C.-T. Yip, L. Wang, H. Huang, L. Zhou*

Hydrogenated TiO_2 Nanotube Arrays as High-Rate Anodes for Lithium-Ion Microbatteries

Battery powered: Annealing under a reducing atmosphere (5% H_2 and 95% Ar) has considerably improved the high-rate capability of TiO_2 nanotube arrays, which have been applied as anodes for lithium-ion microbatteries. This improvement is attributed to the increased bulk electronic conductivity, making the TiO_2 nanotubes favor a bulk n-type conductor (see figure).

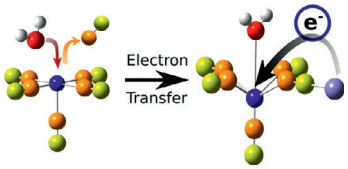


Photomagnetic Prussian Blue

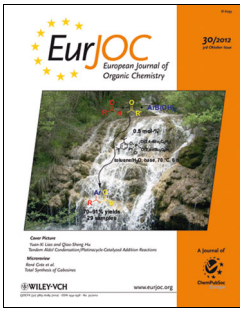
T. Krah,* N. Suaud, A. Zanchet, V. Robert, N. Ben Amor*

Vacancy-Induced Deformation in a CoFe Prussian Blue Analogue – A Theoretical Investigation

On the route towards a better understanding of the photomagnetic properties of the CoFe Prussian Blue analogue, the impact of vacancy-induced deformations and alkali cations on the electronic structure of the embedded $[Co(NC)_5(H_2O)]^{2-}$ cluster were investigated by ab initio quantum chemistry calculations.



Eur. J. Inorg. Chem.
DOI: **10.1002/ejic.201200857**

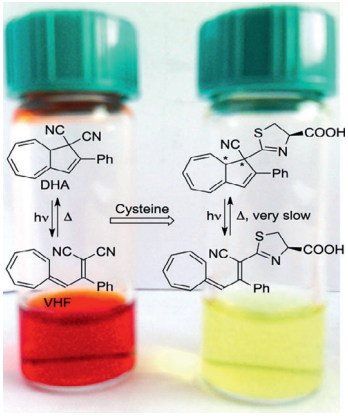


Thiol Chemodosimeter

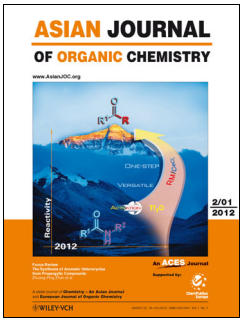
M. Cacciarini,* E. A. Della Pia, M. B. Nielsen

Colorimetric Probe for the Detection of Thiols: The Dihydroazulene/Vinylheptafulvene System

Can the dihydroazulene/vinylheptafulvene (DHA/VHF) photo/thermoswitch system be used as a chemodosimeter for thiols? A new application for this versatile system has been discovered.



Eur. J. Org. Chem.
DOI: **10.1002/ejoc.201200887**

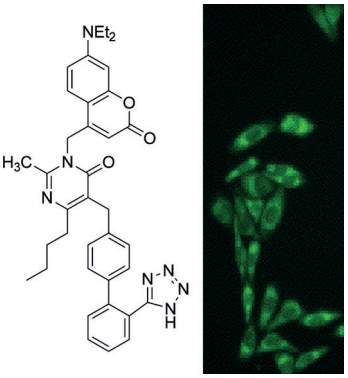


AT1 Receptor Antagonists

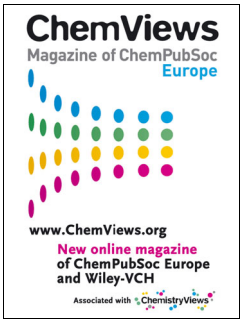
M. A. Giarrusso, M. K. Taylor, J. Ziogas, K. M. Brody, P. E. Macdougall, C. H. Schiesser *

Fluorescent Angiotensin AT_1 Receptor Antagonists

Molecules of a sartan nature: Fluorescent selective angiotensin AT_1 receptor antagonists (sartans) have been prepared and their pharmacology evaluated in Chinese hamster ovary (CHO) cell based assays. Preliminary imaging studies on using these compounds as probes for the localisation of AT_1 receptors in cells are also presented.



Asian J. Org. Chem.
DOI: **10.1002/ajoc.201200064**



Supramolecular Chemistry

Vera Köster

Nanomaterials and Chocolate – Interview with Luisa De Cola

Professor Luisa De Cola recently moved from the University of Münster, Germany, to the ISIS in Strasbourg, France, to accept the chair in supramolecular chemistry. In an interview she talks about her international career so far, how she chose the interdisciplinary area of nanomaterials as her research field, the increasing role of the internet in teaching, and her love of cinema and chocolate.

ChemViews magazine
DOI: **10.1002/chemv.201200091**