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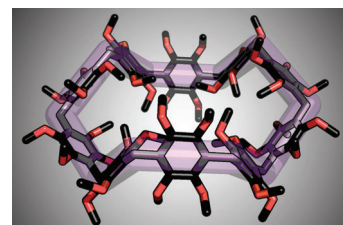


Supramolecular Chemistry

S. T. Schneebeli, C. Cheng, K. J. Hartlieb, N. L. Strutt, A. A. Sarjeant, C. L. Stern, J. F. Stoddart*

Asararenes—A Family of Large Aromatic Macrocycles

Gingering up macrocycles: Asarol methyl ether (1,2,4,5-tetramethoxybenzene), a component of ginger, reacts with paraformaldehyde in the presence of $\text{BF}_3 \cdot \text{OEt}_2$ to produce a new family of macrocycles. Solid-state structures of asar[6]-, asar[7]-, asar[8]-, asar[9]-, asar[10]- and asar[11]arene shed light on the conformational behavior of this new family of potential receptors, which could find applications in materials science and the life sciences in the fullness of time.



Chem. Eur. J.
DOI: 10.1002/chem.201204097

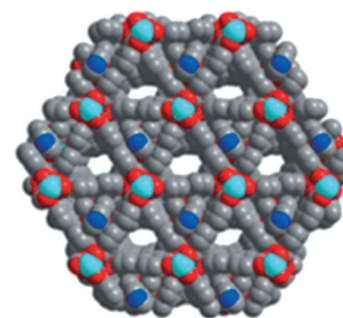


Gas Adsorption

H. Liu, Y. Zhao, Z. Zhang, N. Nijem, Y. J. Chabal, X. Peng, H. Zeng,* J. Li*

Ligand Functionalization and Its Effect on CO_2 Adsorption in Microporous Metal–Organic Frameworks

One up, one down: Functionalization of metal–organic framework structures by a methyl group leads to two opposing and competitive effects on CO_2 adsorption: enhanced CO_2 affinity and reduced porosity.



Chem. Asian J.
DOI: 10.1002/asia.201201081

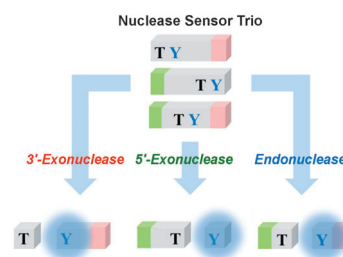


Sensors

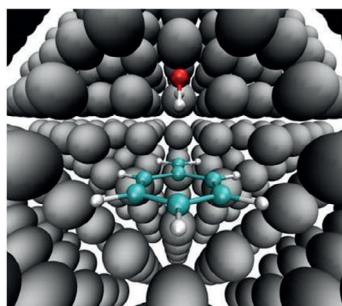
J.-W. Jung, S. K. Edwards, E. T. Kool*

Selective Fluorogenic Chemosensors for Distinct Classes of Nucleases

Nuclease sensor trio: Fluorogenic DNA sensors were developed for distinct classes of nucleases: 3'-exonucleases, 5'-exonucleases, and endonucleases. The highly selective sensors, built from very small modified DNA oligomers containing the unnatural fluorescent base pyrene, and employing thymine as a quencher, were found to function in a variety of complex biological media.



ChemBioChem
DOI: 10.1002/cbic.201300001



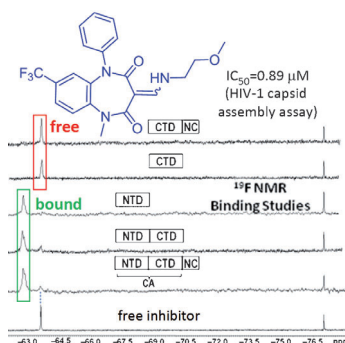
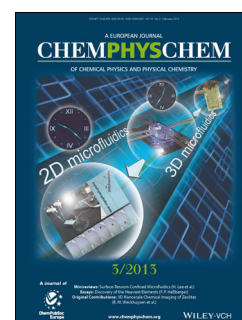
ChemPhysChem
DOI: 10.1002/cphc.201200840

Water-Radical Complexes

R. Crespo-Otero, K. Bravo-Rodriguez, S. Roy, T. Benighaus, W. Thiel, W. Sander, E. Sánchez-García*

Interactions of Aromatic Radicals with Water

Complex radical interactions: The complexes of aromatic radicals and water are investigated using computational methods (see picture) and (for the benzyl radical–water complex) by matrix isolation experiments.



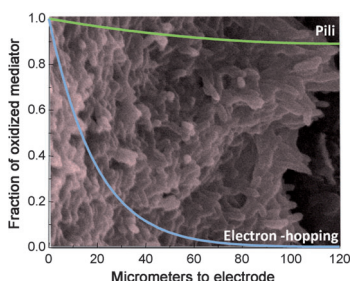
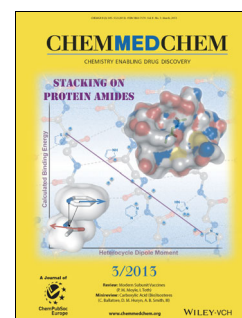
ChemMedChem
DOI: 10.1002/cmdc.201200580

Drug Development

N. Goudreau,* R. Coulombe,* A.-M. Faucher, C. Grand-Maître, J.-E. Lacoste, C. T. Lemke, E. Malenfant, Y. Bousquet, L. Fader, B. Simoneau, J.-F. Mercier, S. Titolo, S. W. Mason

Monitoring Binding of HIV-1 Capsid Assembly Inhibitors Using ^{19}F Ligand- and ^{15}N Protein-Based NMR and X-ray Crystallography: Early Hit Validation of a Benzodiazepine Series

CA all the way! Early hits from a series of benzodiazepine inhibitors of viral capsid protein (CA), a novel target against HIV, were characterized using NMR and X-ray co-crystallography. Ligand-based ^{19}F NMR was used to confirm binding specificity and reversibility, and to identify the N-terminal domain (CA_{NTD}) as the molecular target. Protein-based NMR identified key residues involved in binding, while X-ray co-crystallography confirmed the binding site and mode. Conformationally restricted cyclic inhibitors further validated the possible binding modes.



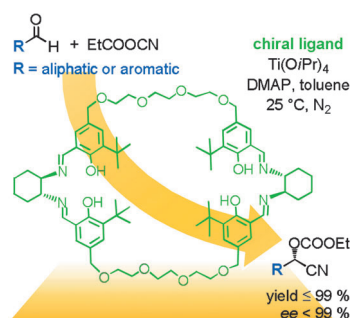
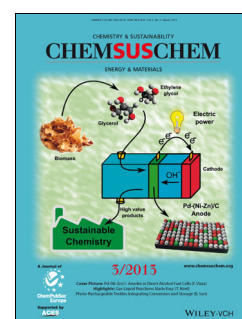
ChemSusChem
DOI: 10.1002/cssc.201200671

Microbial Fuel Cells

P. S. Bonanni,* D. F. Bradley, G. D. Schrott, J. P. Busalmen

Limitations for Current Production in *Geobacter sulfurreducens* Biofilms

Hop, skip, and jump: A mathematical model that allows the identification of limiting steps for current production under several experimental conditions and in different layers of a biofilm is presented. A comparison of model outputs considering electron hopping and conduction through pili indicates that only electron hopping can account for some recent experimental results.



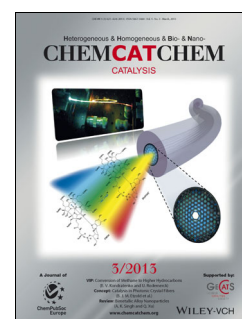
ChemCatChem
DOI: 10.1002/cctc.201200617

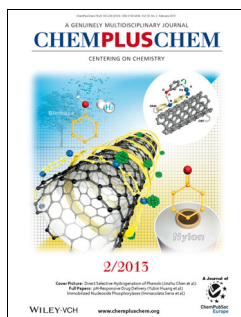
Asymmetric Carbonylation

A. Sadhukhan, M. K. Choudhary, N.-u. H. Khan,* R. I. Kureshy, S. H. R. Abdi, H. C. Bajaj

Asymmetric Cyanoethoxy Carbonylation Reaction of Aldehydes Catalyzed by a Ti^{IV} Macrocyclic Complex: An Efficient Synthetic Protocol for β -Blocker and α_1 -Adrenergic Receptor Agonists

A crown of titanium: A new class of chiral macrocyclic Ti^{IV} –salen complexes are efficient, recyclable, and scalable catalysts for the asymmetric addition of ethyl cyanoformate to aldehydes, which is useful for the synthesis of bioactive compounds. The figure shows the best-performing ligand with two salen units linked flexibly in a crown ether-like motif.



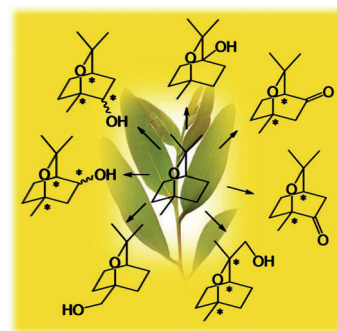


Enzyme Catalysis

M. Schaffarczyk, T. S. Balaban, M. Rychlik, A. Buettner*

Syntheses of Chiral 1,8-Cineole Metabolites and Determination of Their Enantiomeric Composition in Human Urine After Ingestion of 1,8-Cineole-Containing Capsules

Biotransformation of odorants and volatiles in humans is essential for understanding their potential roles with regard to physiological action. Eucalyptol, a common odorant, is shown to yield a range of chiral metabolites that are detectable in human urine, thereby revealing information on rarely investigated pathways in human metabolism (see figure).



ChemPlusChem
DOI: 10.1002/cplu.201200253

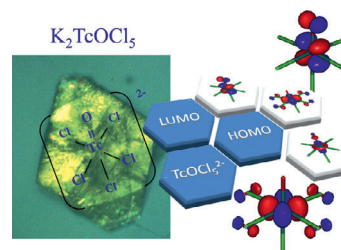


Technate Complex Anions

E. V. Johnstone,* P. F. Weck, F. Poineau, E. Kim, P. M. Forster, A. P. Sattelberger, K. R. Czerwinski

X-ray Crystallographic and First-Principles Theoretical Studies of $K_2[TcOCl_5]$ and UV/Vis Investigation of the $[TcOCl_5]^{2-}$ and $[TcOCl_4]^{-}$ Ions

Dipotassium pentachloridooxidotechnetate has been isolated as single crystals and its structure investigated by crystallographic and first-principles theoretical techniques.



Eur. J. Inorg. Chem.
DOI: 10.1002/ejic.201201346

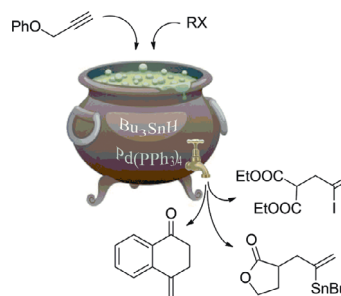


One-Pot Reaction

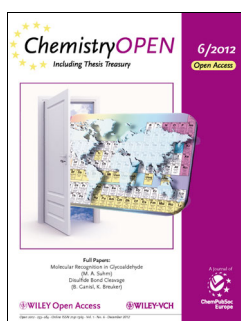
M. R. Klos, U. Kazmaier*

A Catalyst-Economic One-Pot Protocol for the Synthesis and Conversion of Functionalized Vinylstannanes

A wide range of functionalized compounds can easily be obtained by a Pd-catalyzed one-pot hydrostannylation/elimination/distannylation/radical allylation sequence. In this highly catalyst-economic protocol, the Pd catalyst can be involved in up to 5 different reactions.



Eur. J. Org. Chem.
DOI: 10.1002/ejoc.201201593

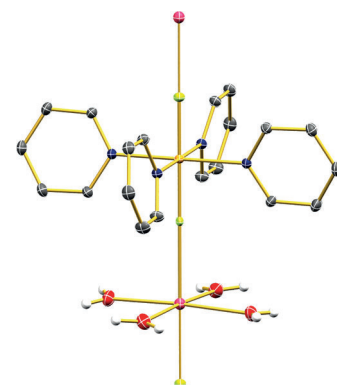


Thesis Treasury

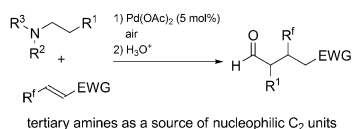
T. Birk*

Fluoride as Ligand: Chemistry of Some New Terminal and Bridged Systems

Fluorine is unique! A synthesis method for polynuclear systems with bridging fluorido ligands has been developed. The method is based on anchoring and protection of the fluorido ligand by initial coordination to a robust metal center (e.g., Cr^{III}) and subsequent use of the robust fluoride complex for construction of more complicated polynuclear structures.



ChemistryOpen
DOI: 10.1002/open.201200046



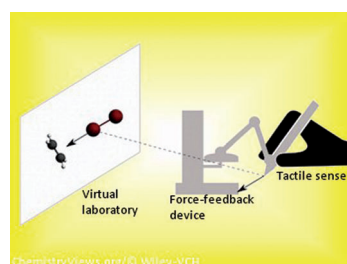
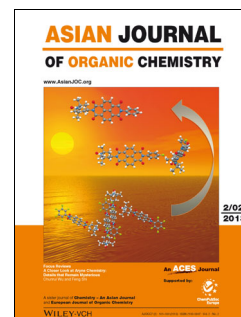
Asian J. Org. Chem.
DOI: 10.1002/ajoc.201300007

Synthetic Methods

A. Morigaki, M. Kawamura, S. Arimitsu, T. Ishihara, T. Konno*

Application of Tertiary Amines Synthesized by Catalytic Dehydrogenation of Enamines as Nucleophilic C₂ Synthons for 1,4-Conjugate Addition with Fluoroalkylated Olefins

The **synthesis** of enamines from only tertiary amines has been developed by using a catalytic amount of Pd(OAc)₂ (5 mol%) in air. These generated enamines were successfully used for 1,4-conjugated addition reactions with fluoroalkylated olefins as an alternative synthetic route for the formylmethylation of olefins. This reaction adds potential for the use of tertiary amines as a nucleophilic C₂ synthon. EWG = electron-withdrawing group.



ChemViews magazine
DOI: 10.1002/chemv.201300006

Quantum Chemistry

V. Köster

Feel Your Molecule's Reactions

Quantum chemistry might soon revolutionize the understanding of reaction pathways. Markus Reiher, ETH Zurich, and colleagues work to combine haptic devices and fast quantum mechanical calculations of attractive and repulsive forces to make you feel in real time the preferred path of a reaction. All you have to do is move one molecule towards another with a pen of a haptic device.

