

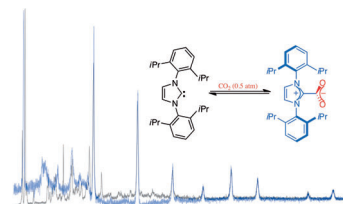


Carbenes

M. Vogt, J. E. Bennett, Y. Huang, C. Wu, W. F. Schneider,*
J. F. Brennecke,* B. L. Ashfeld*

Solid-State Covalent Capture of CO₂ by Using N-Heterocyclic Carbenes

Capture me! The first report of a N-heterocyclic carbene (NHC) as a solid-state carbon capture reagent is presented. Experimental and theoretical measurements demonstrate the ability of the NHC to react rapidly and stoichiometrically with CO₂ at low partial pressures (see scheme).



Chem. Eur. J.
DOI: 10.1002/chem.201302013

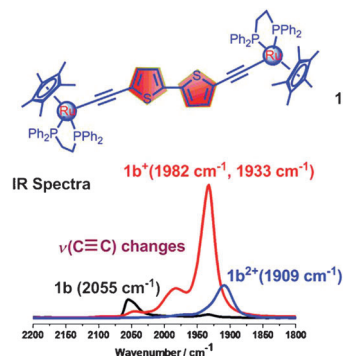


Bimetallic Complexes

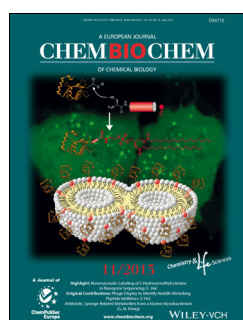
Y.-P. Ou, J. Xia, J. Zhang, M. Xu, J. Yin, G.-A. Yu, S. H. Liu*

Experimental and Theoretical Studies of Charge Delocalization in Biruthenium-Alkynyl Complexes Bridged by Thiophenes

Bridge over troubled waters: A series of binuclear ruthenium-alkynyl complexes that were bridged by thiophene groups have been synthesized and characterized. A combined experimental and computational study suggested that all of these bimetallic ruthenium complexes displayed redox non-innocent ligand behavior.



Chem. Asian J.
DOI: 10.1002/asia.201300419

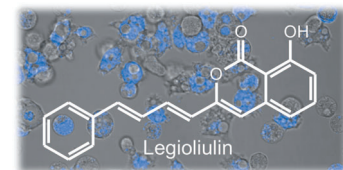


Biosynthesis

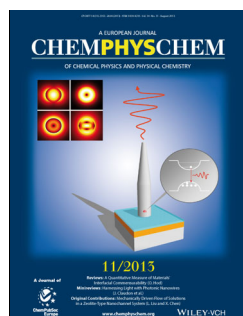
T. Ahrendt, M. Miltenberger, I. Haneburger, F. Kirchner,
M. Kronenwerth, A. O. Brachmann, H. Hilbi, H. B. Bode*

Biosynthesis of the Natural Fluorophore Legiolulin from *Legionella*

Let it shine: The biosynthesis of the UV fluorophore legiolulin (**1**) from *Legionella* spp. was elucidated and the phenylalanine ammonium lyase LglD responsible for the formation of the starter unit cinnamic acid was biochemically characterized. Additionally, two novel derivatives differing in the starter unit have been identified by mutasynthesis experiments.



ChemBioChem
DOI: 10.1002/cbic.201300373

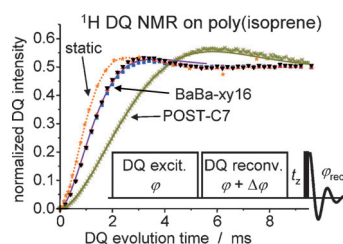


Dipolar Coupling

K. Saalwächter*

Robust NMR Approaches for the Determination of Homonuclear Dipole–Dipole Coupling Constants in Studies of Solid Materials and Biomolecules

Between the poles: The use of different strategies to account for intensity loss in homonuclear double-quantum nuclear magnetic resonance experiments for dipolar coupling quantification is discussed, stressing the use of intensity normalization through a separately measured reference intensity. Similarities to the heteronuclear case of rotational-echo double-resonance experiments are pointed out, and comparisons are made with alternative constant-time approaches.



ChemPhysChem
DOI: 10.1002/cphc.201300254



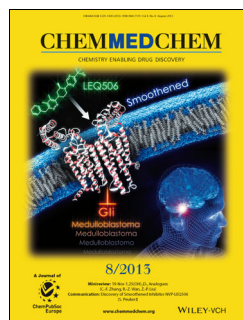
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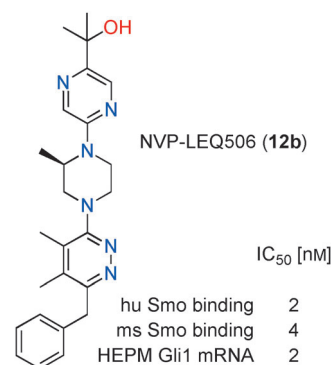


Drug Discovery

S. Peukert,* F. He, M. Dai, R. Zhang, Y. Sun, K. Miller-Moslin, M. McEwan, B. Lagu, K. Wang, N. Yusuff, A. Bourret, A. Ramamurthy, W. Maniara, A. Amaral, A. Vattay, A. Wang, R. Guo, J. Yuan, J. Green, J. Williams, S. Buonamici, J. F. Kelleher, III, M. Dorsch

Discovery of NVP-LEQ506, a Second-Generation Inhibitor of Smoothed

First disclosure: Continued optimization provided a novel type of Smoothed (Smo) antagonist based on a pyridazine core. The compound, NVP-LEQ506, currently in phase I clinical trials, combines high intrinsic potency and good pharmacokinetic properties resulting in excellent efficacy in rodent tumor models of medulloblastoma. Activity against a Smo mutant conferring resistance observed in a previous clinical trial with a competitor compound suggests additional therapeutic potential.



ChemMedChem
DOI: 10.1002/cmdc.201300217

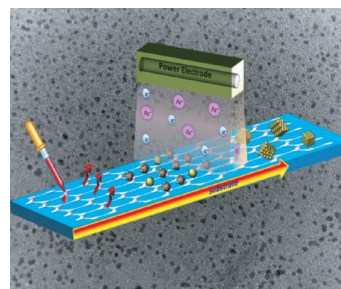


Solar Cells

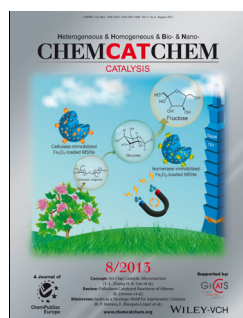
V.-D. Dao, L. V. Nang, E.-T. Kim, J.-K. Lee, H.-S. Choi*

Pt Nanoparticles Immobilized on CVD-Grown Graphene as a Transparent Counter Electrode Material for Dye-Sensitized Solar Cells

Crystal clear: Dry plasma reduction is used for continuously immobilizing platinum nanoparticles on CVD-grown graphene under atmospheric pressure without using any toxic chemicals while keeping the temperature low. The PtNPs/graphene-coated counter electrode exhibits a reasonably low charge-transfer resistance and a high optical transmittance.



ChemSusChem
DOI: 10.1002/cssc.201300353

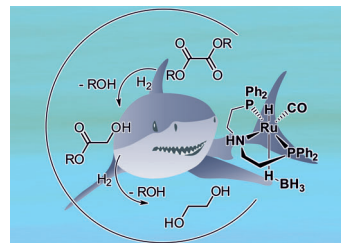


Hydrogenation

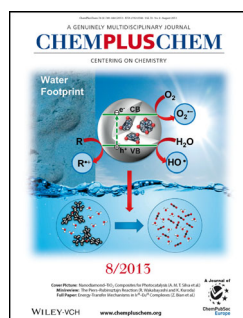
C. Ziebart, R. Jackstell, M. Beller*

Selective Catalytic Hydrogenation of Diethyl Oxalate and Related Esters

Ruthenium shark takes a bite: Oxalic acid esters are smoothly hydrogenated into either alkyl glycolate or ethylene glycol under mild conditions.



ChemCatChem
DOI: 10.1002/cctc.201300209

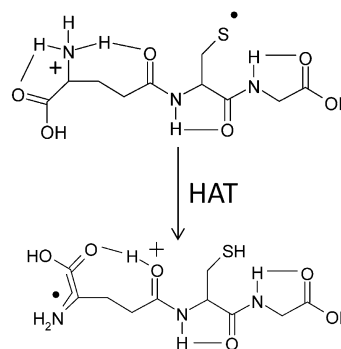


Radical Rearrangements

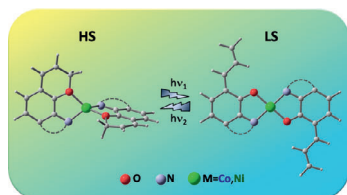
S. Osburn, G. Berden, J. Oomens, K. Gulyuz, N. C. Polfer, R. A. J. O'Hair, V. Ryzhov*

Structure and Reactivity of the Glutathione Radical Cation: Radical Rearrangement from the Cysteine Sulfur to the Glutamic Acid α -Carbon Atom

Totally radical: Gas-phase ion-molecule reactions were used to observe a radical rearrangement in the radical cation of glutathione (see scheme). This rearrangement proceeded from sulfur to the glutamic acid α -carbon atom, which was confirmed by infrared multiple photon dissociation (IRMPD) spectroscopy in two different IR regions (1000–1800 and 2800–3700 cm⁻¹) and DFT calculations.



ChemPlusChem
DOI: 10.1002/cplu.201300057



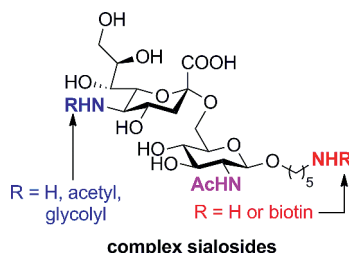
Eur. J. Inorg. Chem.
DOI: 10.1002/ejic.201300264

Spin Crossover

A. A. Starikova, R. M. Minyaev, A. G. Starikov, V. I. Minkin*

DFT Computational Design of a Ligand-Driven Light-Induced Mechanism for Spin-State Switching

B3LYP*/6-311++G(d,p) DFT calculations have been performed on a series of bis-chelate four-coordinate Co^{II}, Ni^{II}, and Cu^{II} complexes of photochromic 2*H*-chromene ligands. In the case of the Ni^{II} complexes, the light-driven electrocyclic rearrangements of the ligand moieties lead to sharp switching of the spin states of the complexes.



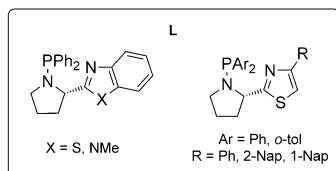
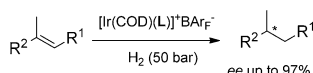
Eur. J. Org. Chem.
DOI: 10.1002/ejoc.201300664

Sialoside Synthesis

T. J. Boltje,* T. Heise, F. P. J. T. Rutjes, F. L. van Delft

A Divergent Method to Prepare 5-Amino-, 5-*N*-Acetamido-, and 5-*N*-Glycolysialosides

A major determinant of sialic acid recognition is the N-5 substituent, which can be an *N*-acetyl (human), *N*-glycolyl (non-human), or amine (cancer associated) functionality. Herein, we report a divergent chemical approach to enable the synthesis of the aforementioned 5-*N*-substituted sialosides by using a single sialic acid building block.



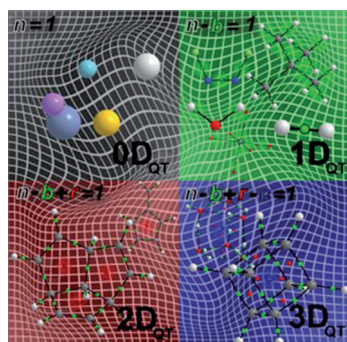
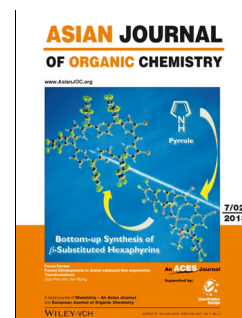
Asian J. Org. Chem.
DOI: 10.1002/ajoc.201300045

Asymmetric Hydrogenation

N. Yotapan, A. Paptchikhine, M. Bera, S. K. Avula, T. Vilaivan,* P. G. Andersson*

Simple Proline-Derived Phosphine-Thiazole Iridium Complexes for Asymmetric Hydrogenation of Trisubstituted Olefins

Talkin' 'bout hydrogenation: Proline-based phosphine-thiazole/imidazole ligands are effective ligands for homogeneous, iridium-catalyzed, asymmetric hydrogenation of trisubstituted functionalized and unfunctionalized olefins.



ChemViews magazine
DOI: 10.1002/chemv.201300080

Graphene

Samantha Jenkins and Matteo Cavalleri

Is Graphene Really a 2D Material?

Graphene is often described as a two-dimensional material. But graphene sheets can contain waves as distortions because the carbon rings are puckered. Professor Samantha Jenkins, Hunan Normal University, China, looks at a way to describe dimensionality in terms of the Quantum Theory of Atoms in Molecules (QTAIM) to settle the debate.

