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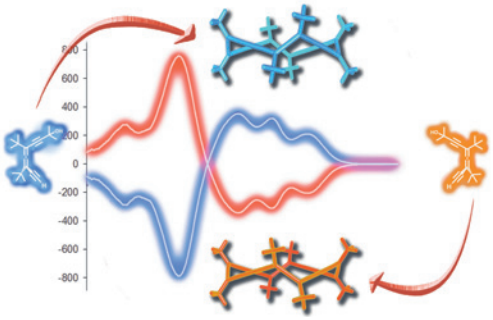
Swiss Science Concentrates

A CHIMIA Column

Short Abstracts of Interesting Recent Publications of Swiss Origin

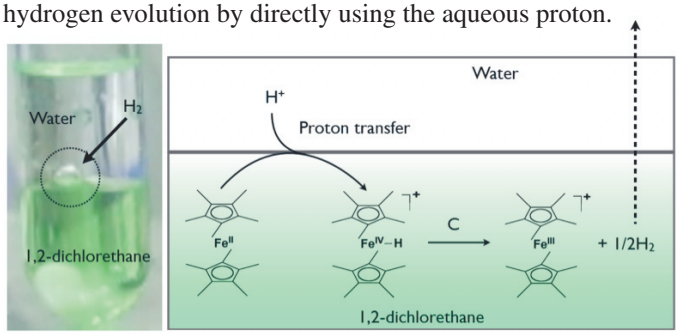
An Enantiomerically Pure Alleno-Acetylenic Macrocycle: Synthesis and Rationalization of Its Outstanding Chiroptical Response

J. L. Alonso-Gómez, P. Rivera-Fuentes, N. Harada, N. Berova, and F. Diederich*, *Angew. Chem., Int. Ed.* **2009**, *48*, 5545
ETH Zürich, Columbia University and Tohoku University
While strained small-ring allenes have been investigated in greater detail for their theoretical properties and their limits of stability and isolability, allenic macrocycles, in particular shape-persistent ones, are mostly unknown. In this paper, the first enantiomerically pure alleno-acetylenic macrocycles (*P*,*P*,*P*,*P*)-(–)-**1** (red) and (*M*,*M*,*M*,*M*)-(+)-**1** (blue) were synthesized from enantiopure 1,3-di-*tert*-butyl-1,3-diethynylallenes. A remarkable magnitude of the Cotton effects in the circular dichroism spectra was noticed which can be explained by a unique combination of geometric and electronic properties.



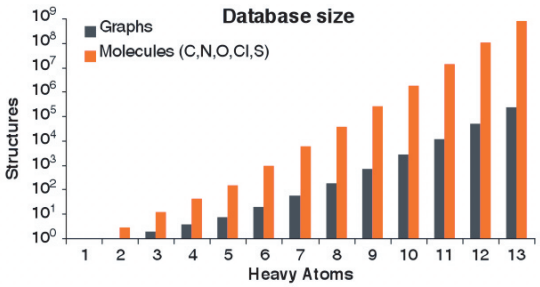
Hydrogen Evolution at Liquid–Liquid Interfaces

I. Hatay, B. Su, F. Li, R. Partovi-Nia, H. Vrubel, X. Hu, M. Ersoz, and H. H. Girault*, *Angew. Chem., Int. Ed.* **2009**, *48*, 5139
EPFL, Lausanne University and Selcuk University, Turkey
In this article, the authors describe a novel hydrogen evolution reaction at a soft immiscible interface of an aqueous acidic solution and an immiscible organic solvent (1,2-dichloroethane: DCE) containing [$(C_5Me_5)_2Fe$] as an electron donor. The reaction proceeds by proton transfer assisted by the ferrocene complex across the water-DCE interface with subsequent proton reduction in DCE. The interface essentially acts as a proton pump, allowing hydrogen evolution by directly using the aqueous proton.



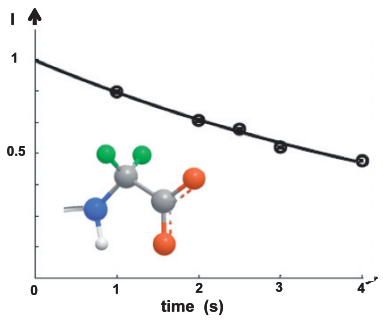
970 Million Druglike Small Molecules for Virtual Screening in the Chemical Universe Database GDB-13

L. C. Blum and J.-L. Reymond*, *J. Am. Chem. Soc.* **2009**, *131*, 8732
University of Bern
One of the most important chemical issues in drug discovery is innovation, in particular at the level of small organic fragments that can provide new lead structures. In this article, the authors present the new chemical database GDB-13, which enumerates 977 468 314 structures of small molecules containing up to 13 atoms of C, N, O, S and Cl. GDB-13 is the largest publicly available database of virtual small molecules. It is freely available for download at *http://www.gdb.unibe.ch.*



Diffusion Coefficients of Biomolecules Using Long-Lived Spin States

P. Ahuja, R. Sarkar, P. R. Vasos*, and G. Bodenhausen, *J. Am. Chem. Soc.* **2009**, *131*, 7498
EPF Lausanne, Ecole Normale Supérieure, Paris
In this paper, the authors described the first observation of long-lived spin states (LLS) of aliphatic protons belonging to amino acids in a protein having lifetimes T_{LLS} that exceed the corresponding spin-lattice relaxation times T_1 by more than a factor 6. Slow diffusion coefficients characteristic of large biomolecules can be determined by combining LLS methods with moderate pulsed field gradients (PFGs) available on commercial probeheads, as the extension of spin memory reduces the strain on the duration and/or strength of the PFGs. No isotope labeling of the biomolecule is necessary.



Prepared by M. Austeri, R. Bach, J. Guin, A. Sharma, F. Toricelli, W. Zeghida, J. Lacour
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