Top-Beiträge ...

Vinylidenes

B. M. Trost,* A. McClory

Metal Vinylidenes as Catalytic Species in Organic Reactions

It's a very useful thing: Metal vinylidenes may be accessed through transitionmetal activation of terminal alkynes. This Focus Review addresses the reactions that these electrophilic species undergo as well as their application in organic synthesis.

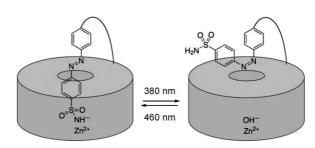
Chem. Asian J.

DOI: 10.1002/asia.200700247

Photoaffinity Labeling

J. H. Harvey, D. Trauner*

Regulating Enzymatic Activity with a Photoswitchable Affinity Label



Best PALs: We have applied a photoswitchable affinity label (PAL) to the optical control of protein function. The enzymatic activity of native carbonic anhydrase was controlled with covalently tethered, photoswitchable inhibitors (see scheme). This system allows the photoregulation of native proteins without site-specific introduction of highly reactive residues.

ChemBioChem

DOI: 10.1002/cbic.200700570

Internal Rotations

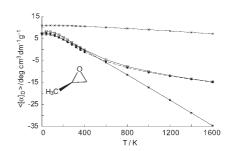
B. C. Mort, J. Autschbach*

A Pragmatic Recipe for the Treatment of Hindered Rotations in the Vibrational Averaging of Molecular Properties

Chem Phys Chem

DOI: 10.1002/cphc.200700628

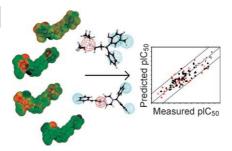
Effects of internal rotations: A computational procedure to treat hindered rotations in the vibrational averaging of molecular properties and their temperature dependence is undertaken. The figure shows the impact of the hindered rotation of the methyl group in (R)-methyloxirane on the optical rotation as a function of temperature.



QSAR Models

C. Kramer, B. Beck,* J. M. Kriegl, T. Clark*

A Composite Model for hERG Blockade



hERG blockade is one of the major toxicological problems in lead structure optimization. We present a predictive QSAR model for hERG blockade that differentiates between specific and nonspecific binding by preliminary pharmacophore scanning. While PLS and SVR models reach competitive R² values, the mixture of interpretable quantum mechanically derived descriptors and pharmacophorebased splits of the datasets offers a novel approach toward the understanding of hERG blockade.

ChemMedChem

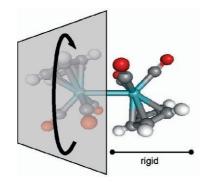
DOI: 10.1002/cmdc.200700221



... aus unseren Schwesterzeitschriften



The motion of $FeCp(CO)_2X$ (where X =I, CH₃) and Mo₂Cp₂(CO)₆ complexes included in β - or γ -cyclodextrin was studied by comparing the ¹³C CPMAS NMR spectra of the adducts with that of FeCp(CO)₂X and Mo₂Cp₂(CO)₆, respectively. The nature of the motion was shown to be dependent on the symmetry, size and orientation of the guest molecule within the host cavity.



Mobility in Cyclodextrins

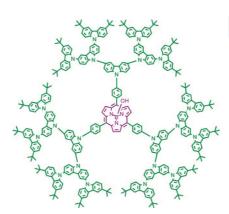
S. Aime, M. R. Chierotti, R. Gobetto,* A. Masic, F. Napolitano, H. C. Canuto,

Intramolecular Host-Guest Dynamics of $FeCp(CO)_2X$ (X = I and CH₃) and $Mo_2Cp_2(CO)_6$ Included in β - or γ-Cyclodextrin

Eur. J. Inorg. Chem.

DOI: 10.1002/ejic.200700799

Novel dendritic carbazole-functionalized subporphyrins have been synthesized from pyridine-tri(pyrrol-1-yl)borane and the corresponding aldehydes. In these molecules, efficient photoinduced intramolecular energy transfer occurs from the carbazole dendron to the subporphyrin core. The carbazole dendron can significantly influence the absorption and emission spectra of the subporphyrin core, which are blueshifted with increasing dendron generation.



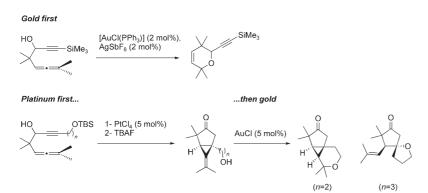
Dendritic Subporphyrins

T. Xu, R. Lu,* X. Liu, P. Chen, X. Qiu, Y. Zhao

Synthesis and Characterization of Subporphyrins with Dendritic Carbazole

Eur. J. Org. Chem.

DOI: 10.1002/ejoc.200700981



Gamble on gold or platinum? Hydroxylated 1,5-allenynes can be cycloisomerized to dihydropyrans by an allenophilic Au catalyst. On the other hand, 6methylenebicyclo[3.1.0]hexan-3-ones were formed after selective alkynophilic Pt-catalyzed cycloisomerization. The methylenecyclopropane moiety can in turn be activated by Au¹, with formation of tricyclic compounds resulting from the nucleophilic attack of the double bond or spiro derivatives resulting from the nucleophilic attack of the cyclopropyl ring (see scheme).

Homogeneous Catalysis

R. Zriba, V. Gandon, C. Aubert, L. Fensterbank,* M. Malacria*

Alkyne versus Allene Activation in Platinum- and Gold-Catalyzed Cycloisomerization of Hydroxylated 1,5-Allenynes

Chem. Eur. J.

DOI: 10.1002/chem.200701522

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