

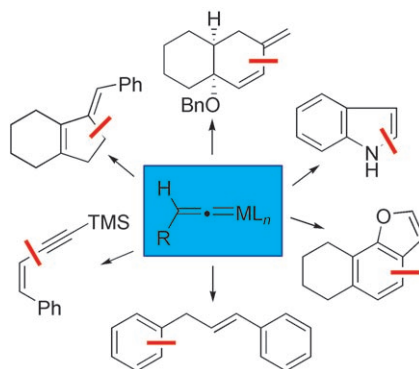
Vinylidenes

B. M. Trost,* A. McClory

Metal Vinylidenes as Catalytic Species in Organic Reactions

Chem. Asian J.

DOI: 10.1002/asia.200700247



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

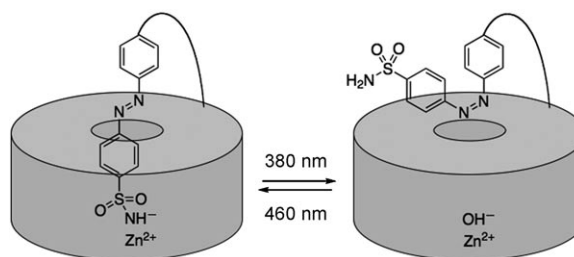
Photoaffinity Labeling

J. H. Harvey, D. Trauner*

Regulating Enzymatic Activity with a Photoswitchable Affinity Label

ChemBioChem

DOI: 10.1002/cbic.200700570



Best PALs: We have applied a photo-switchable 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 photo-regulation of native proteins without site-specific introduction of highly reactive residues.

Internal Rotations

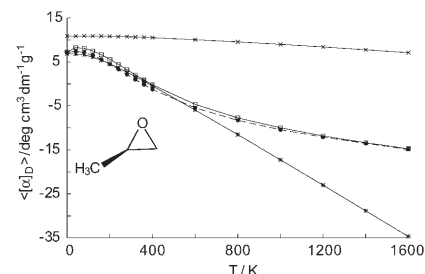
B. C. Mort, J. Autschbach*

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

ChemPhysChem

DOI: 10.1002/cphc.200700628

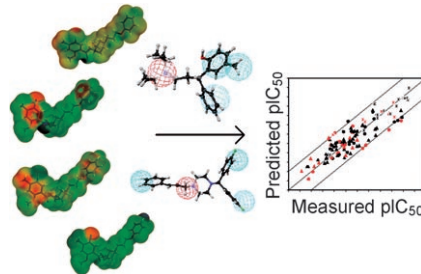
Effects of internal rotations: A computational procedure to treat hindered rotations in the vibrational averaging of molecular properties and their temperature dependence is undertaken. The figure shows the impact of the hindered rotation of the methyl group in (*R*)-methyloxirane on the optical rotation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



QSAR Models

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

A Composite Model for hERG Blockade

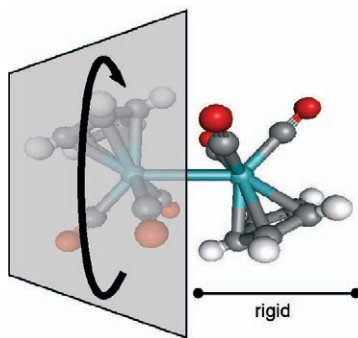


hERG blockade is one of the major toxicological problems in lead structure optimization. We present a predictive QSAR model for hERG blockade that differentiates between specific and nonspecific binding by preliminary pharmacophore scanning. While PLS and SVR models reach competitive R^2 values, the mixture of interpretable quantum mechanically derived descriptors and pharmacophore-based splits of the datasets offers a novel approach toward the understanding of hERG blockade.

ChemMedChem

DOI: 10.1002/cmdc.200700221

The motion of $\text{FeCp}(\text{CO})_2\text{X}$ (where $\text{X} = \text{I}, \text{CH}_3$) and $\text{Mo}_2\text{Cp}_2(\text{CO})_6$ complexes included in β - or γ -cyclodextrin was studied by comparing the ^{13}C CPMAS NMR spectra of the adducts with that of $\text{FeCp}(\text{CO})_2\text{X}$ and $\text{Mo}_2\text{Cp}_2(\text{CO})_6$, 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.



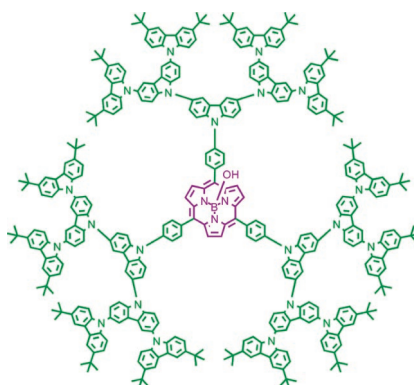
Mobility in Cyclodextrins

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

Intramolecular Host–Guest Dynamics of $\text{FeCp}(\text{CO})_2\text{X}$ ($\text{X} = \text{I}$ and CH_3) and $\text{Mo}_2\text{Cp}_2(\text{CO})_6$ 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.



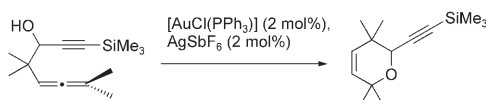
Dendritic Subporphyrins

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

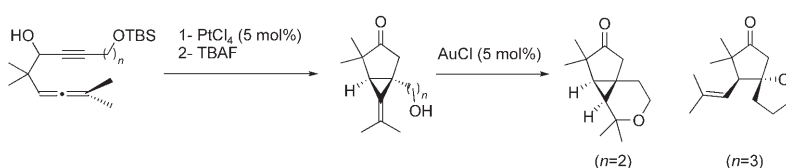
Synthesis and Characterization of Subporphyrins with Dendritic Carbazole Arms

Eur. J. Org. Chem.
DOI: 10.1002/ejoc.200700981

Gold first



Platinum first...



...then gold

Gamble on gold or platinum? Hydroxylated 1,5-allenynes can be cycloisomerized to dihydropyrans by an allenophilic Au^{I} catalyst. On the other hand, 6-methylenebicyclo[3.1.0]hexan-3-ones were formed after selective alkynophilic Pt-catalyzed cycloisomerization. The methyl-

enecyclopropane moiety can in turn be activated by Au^{I} , 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