

SPOTLIGHTS ...

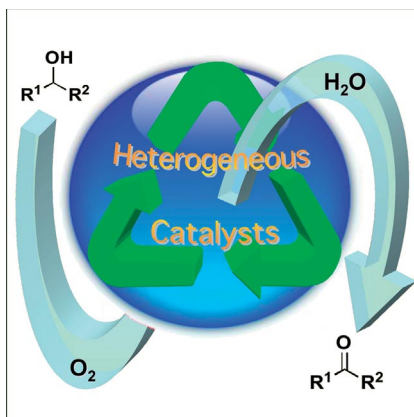
Heterogeneous Catalysts

T. Matsumoto, M. Ueno, N. Wang,
S. Kobayashi*

Recent Advances in Immobilized Metal Catalysts for Environmentally Benign Oxidation of Alcohols

Chem. Asian J.

DOI: 10.1002/asia.200700359



The search is on for heterogeneous catalysts combined with environmentally benign oxidants, such as molecular oxygen and hydrogen peroxide, for the selective oxidation of alcohols. This Focus Review presents an overview of recent developments in immobilized metal catalysts and evaluates the potential of transition metals in the heterogeneously catalyzed oxidation of alcohols.

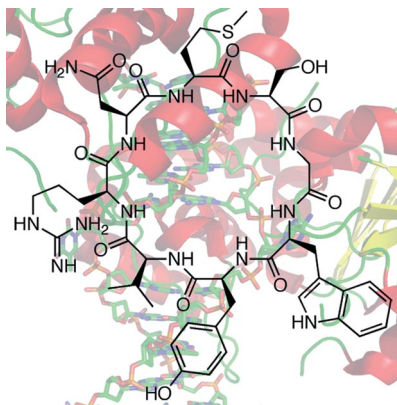
Cyclic Peptides

T. A. Naumann, A. Tavassoli,
S. J. Benkovic*

Genetic Selection of Cyclic Peptide Dam Methyltransferase Inhibitors

ChemBioChem

DOI: 10.1002/cbic.200700561



Let's go round. We report the development of a transposition based genetic selection methodology used to uncover three cyclic peptide inhibitors of the *E. coli* methyltransferase. The activity of the selected cyclic peptides was confirmed in vivo and in vitro. The IC₅₀ of the most active cyclic peptide (SGWYVRNM, shown in the figure) was comparable to that of the known methyltransferase inhibitor, sinefungin.

Optical Activity

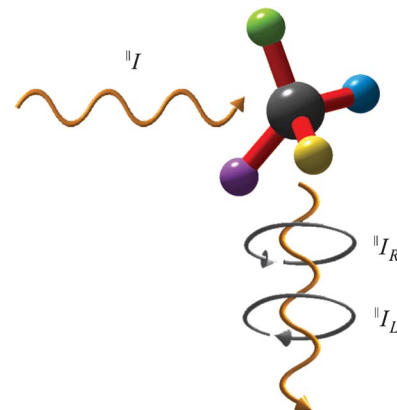
G. Zuber,* P. Wipf,* D. N. Beratan*

Exploring the Optical Activity Tensor by Anisotropic Rayleigh Optical Activity Scattering

ChemPhysChem

DOI: 10.1002/cphc.200700660

Exploring optical activity: Anisotropic RayOA scattering in concert with theoretical analysis provides a powerful new method to assign the absolute configuration of chiral molecules (see picture). Anisotropic RayOA invariants also find applications as chirality descriptors that contain information on both the molecular topology and the electronic structure.



Molecular Modeling

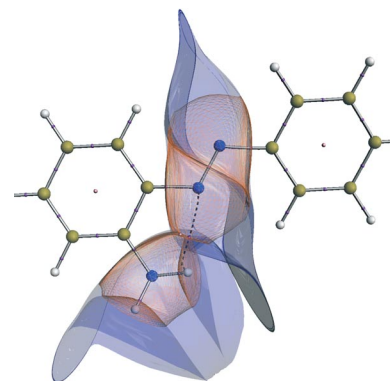
I. Bytheway,* M. G. Darley,
P. L. A. Popelier*

The Calculation of Polar Surface Area from First Principles: An Application of Quantum Chemical Topology to Drug Design

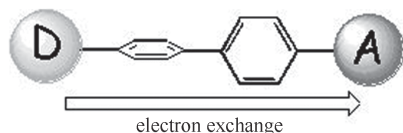
ChemMedChem

DOI: 10.1002/cmdc.200700262

Using QCT for drug design. A newly developed method to calculate the polar surface areas based on quantum chemical topology is described and the results compared with standard methods. Differences between methods showed how the calculation of the PSA depends on the method used, and therefore, judicious application of the upper limits used in the prediction of oral bioavailability is warranted.



... ON OUR SISTER JOURNALS



A new angle on energy transfer: The rate of intramolecular triplet energy transfer in donor-spacer-acceptor dyads (see scheme) depends precisely on the dihedral angle between bridging phenylene rings, but the situation is complicated by mixing with an upper-lying excited triplet state localized on the donor.

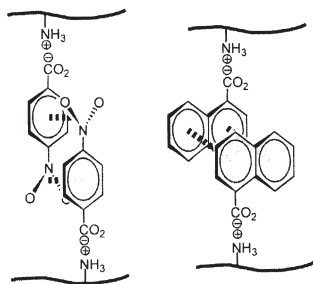
Donor-Acceptor Systems

A. C. Benniston, A. Harriman,* P. Li, P. V. Patel, C. A. Sams

Electron Exchange in Conformationally Restricted Donor-Spacer-Acceptor Dyads: Angle Dependence and Involvement of Upper-Lying Excited States

Chem. Eur. J.

DOI: 10.1002/chem.200701548



Van der Waals interactions between effector molecules in aqueous solution lead to contraction of polyallylamine gel particles, which for benzoic acids increase from about 18% to 70% by the presence of nitro groups, and to 67% with naphthalene derivatives. The observed cooperativity indicates dispersive forces as major driving factor for volume changes in such intelligent materials.

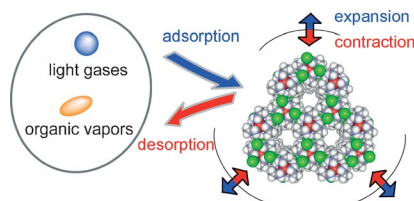
Chemomechanical Polymers

K. Kato, H.-J. Schneider*

Dispersive Effects in Chemomechanical Reactions with Polyallylamine-Derived Hydrogels

Eur. J. Org. Chem.

DOI: 10.1002/ejoc.200700850



Dynamic accommodation: The racemic crystal of (\pm) -[Co(en)₃]Cl₃ (en = ethylenediamine; see space-filling model of lattice: Co red, N blue, Cl green, C gray) includes H₂O molecules within the one-dimensional channels when hydrated. Upon removal of the H₂O molecules by vacuum drying, the crystal exhibits dynamic behavior as a host to a variety of light gases or organic vapors within its channels by expansion/contraction of the lattice while single-crystal properties are maintained.

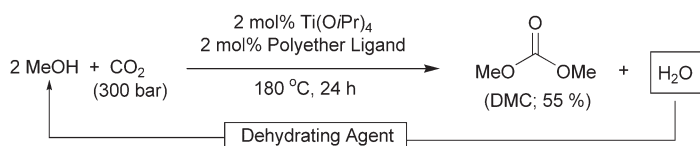
Ionic Crystals

S. Takamizawa,* T. Akatsuka, T. Ueda

Gas-Conforming Transformability of an Ionic Single-Crystal Host Consisting of Discrete Charged Components

Angew. Chem. Int. Ed.

DOI: 10.1002/anie.702950



Run DMC: Homogeneous catalysts based on titanium alkoxides and polyethers were studied for the production of the industrially important intermediate dimethyl carbonate (DMC) from carbon dioxide and methanol

(see scheme). The reaction proceeds in the presence of 2,2-dimethoxypropane as a recyclable organic dehydrating agent under supercritical CO₂ conditions.

Carbon Dioxide Fixation

K. Kohno, J.-C. Choi, Y. Ohshima, H. Yasuda, T. Sakakura*

Synthesis of Dimethyl Carbonate from Carbon Dioxide Catalyzed by Titanium Alkoxides with Polyether-type Ligands

ChemSusChem

DOI: 10.1002/cssc.200700113