Structure–Activity Relationships

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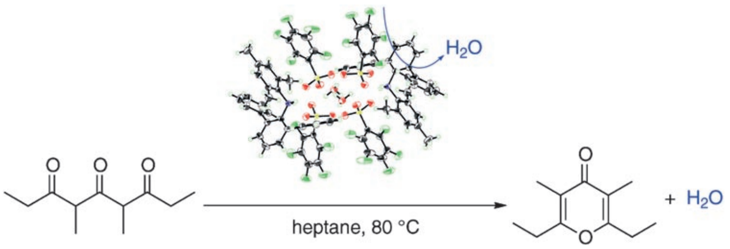
S. Nakagawa, K. Ishihara*

Unusual Rate Acceleration in Brønsted Acid Catalyzed Dehydration Reactions: Local Hydrophobic Environment in Aggregated *N*-(2,6-diphenylphenyl)-*N*-mesitylammonium Pentafluorobenzenesulfonates

Chem. Asian J.
DOI: **10.1002/asia.200600380**



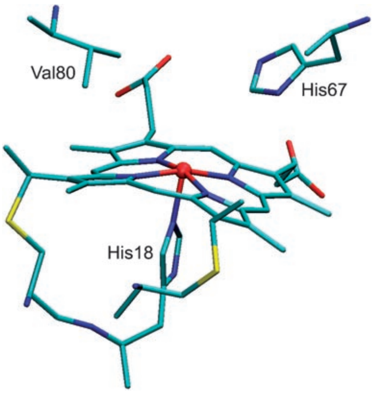
Teaming up for improved efficiency: The hydrophobic environment surrounding the ammonium hydrogen atoms in aggregated $[Ar_2NH_2]^+[O_3SC_6F_5]^-$ catalysts has a significant accelerating effect on the dehydrative cyclization of 1,3,5-triketones (O = red, F = green, N = blue, S = yellow). Dehydration catalysts that do not form a stable cyclic ion pair are less active.

Metalloenzymes

Z.-H. Wang, Y.-W. Lin, F. I. Rosell, F.-Y. Ni, H.-J. Lu, P.-Y. Yang, X.-S. Tan, X.-Y. Li, Z.-X. Huang,* A. G. Mauk*

Converting Cytochrome c into a Peroxidase-Like Metalloenzyme by Molecular Design

ChemBioChem
DOI: **10.1002/cbic.200600547**



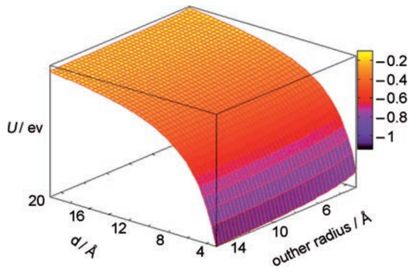
Even better than the real thing. Based on molecular design, an electron-transfer hemoprotein, cytochrome c, was converted into a peroxidase-like enzyme by introduction of a distal histidine into the heme pocket. The cytochrome c variants obtained, Tyr67His and Tyr67His/Met80Val (see figure), showed much higher peroxidase activities than wild-type cytochrome protein. More interestingly, the k_{cat}/K_m values of the new hemoproteins were higher than that of wild-type horseradish peroxidase.

Carbon Nanotubes

E. Bakalis, F. Zerbetto*

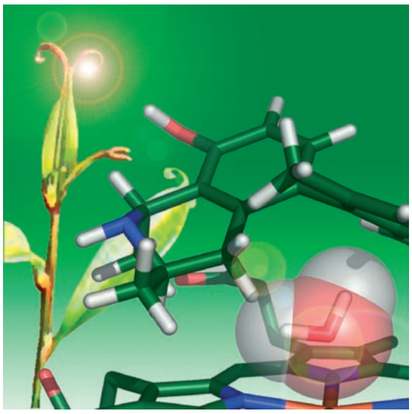
Charge–Metal Interaction of a Carbon Nanotube

ChemPhysChem
DOI: **10.1002/cphc.200600715**



Simple three-dimensional functions: Carbon nanotubes can be semiconducting or metallic and, yet, their interactions with other molecules are often treated as if they were all the same. The authors develop two simple three-dimensional functions that describe the extra energy of interaction of a charge with a metallic nanotube. This energy depends on the radius of the tube and the distance of the charge from either the inner or outer surface of the conducting tube.

Dioncophylline C, a promising antimalarial agent derived from the tropical liana *Triphyophyllum peltatum* is investigated when binding to its presumed target, heme. Structures of the observed complex are calculated from NMR paramagnetic relaxation measurements and the possible mode of complex stabilization is discussed.

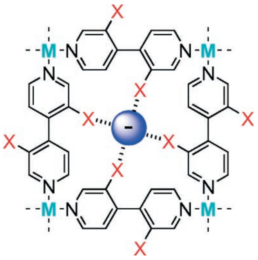


Drug–Target Interactions

K. F. Schwedhelm, M. Horstmann, J. H. Faber, Y. Reichert, G. Bringmann, C. Faber*

The Novel Antimalarial Compound Dioncophylline C Forms a Complex with Heme in Solution

ChemMedChem
DOI: **10.1002/cmdc.200600263**



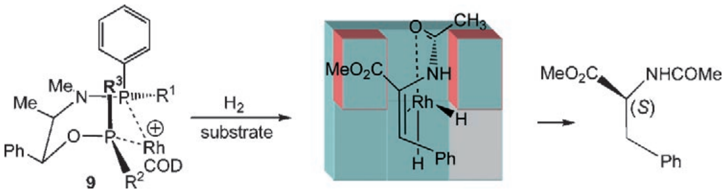
The application of metal–organic frameworks (MOFs) to anion separations with a special emphasis on anion selectivity is reviewed. Non-Hofmeister selectivity and shape recognition are observed in structurally constrained MOFs functionalized with hydrogen-bonding groups.

Anion Separations

R. Custelcean,* B. A. Moyer*

Anion Separation with Metal–Organic Frameworks

Eur. J. Inorg. Chem.
DOI: **10.1002/ejic.200700018**



A series of P-chirogenic AMPP ligands has been synthesized from $(+)$-ephedrine by a versatile three-step methodology and tested in catalyzed hydrogenations of methyl α-acetamidocinnamate by Rh complexes. Variation of the substituent on a P-center of the ligand affords the phenylalanine derivatives with *ee* values ranging from 99% (*S*) to 88% (*R*). A new model for the enantioselectivity, taking into consideration the boat conformation in the AMPP-RhH$_2$ substrate complex, has been proposed.

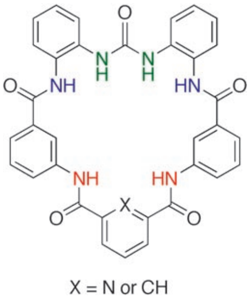
Asymmetric Hydrogenation

C. Darcel,* D. Moulin, J.-C. Henry, M. Lagrelette, P. Richard, P. D. Harvey, S. Jugé*

Modular P-Chirogenic Aminophosphane-Phosphinite Ligands for Rh-Catalyzed Asymmetric Hydrogenation: A New Model for Prediction of Enantioselectivity

Eur. J. Org. Chem.
DOI: **10.1002/ejoc.200600966**

The anion-binding properties of two new hybrid macrocycles (shown here) containing urea and amide hydrogen bond donors has been studied and compared with a series of "fragments" containing various combinations of the hydrogen-bonding motifs present in the macrocyclic systems. The results obtained suggest dramatic differences in the mode of interaction of anions with the two macrocycles.



Macrocycles

S. J. Brooks, S. E. García-Garrido, M. E. Light, P. A. Cole, P. A. Gale*

Conformational Control of Selectivity and Stability in Hybrid Amide/Urea Macrocycles

Chem. Eur. J.
DOI: **10.1002/chem.200601647**