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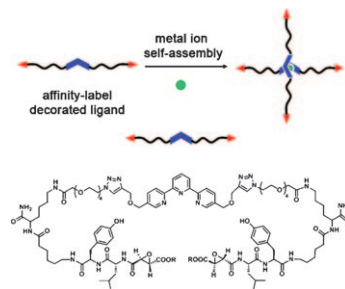


Protein–Inorganic Arrays

N. D. Bogdan, M. Matache, V. M. Meier, C. Dobrotă, I. Dumitru, G. D. Roiban, D. P. Funeriu*

Protein–Inorganic Arrays Construction: Design and Synthesis of the Building Blocks

One step beyond—expanding the size and complexity of supramolecular constructs. We describe the design and synthesis of the first series of di-functional ligands for the directed construction of inorganic–protein frameworks (see scheme). Composed of a metal-ion binding moiety (terpyridine-based) conjugated to an epoxysuccinyl peptide (known to covalently bind active cysteine proteases), the ligands are best synthesized through a click-chemistry approach.



Chem. Eur. J.
DOI: 10.1002/chem.200902649

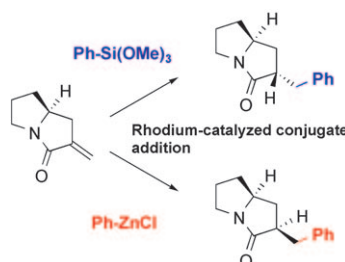


Rhodium Catalysis

J. D. Hargrave, J. C. Allen, C. G. Frost*

Alternatives to Organoboron Reagents in Rhodium-Catalyzed Conjugate Additions

Alternative organometallic donors to organoboron reagents can offer significant advantages in terms of intrinsic reactivity and selectivity, resulting in new transformations for organic synthesis based on rhodium-catalyzed conjugate addition. This Focus Review explores emerging applications in this rapidly expanding area of catalysis.



Chem. Asian J.
DOI: 10.1002/asia.200900512

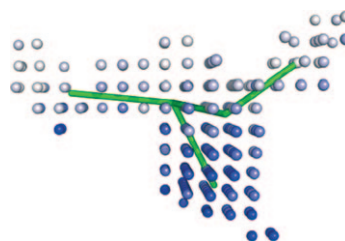


Drug Design

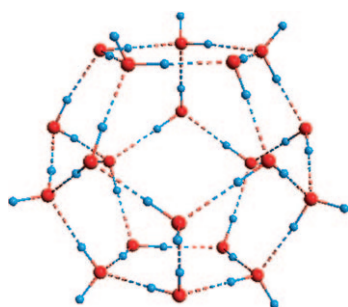
M. Weisel, J. M. Kriegl, G. Schneider*

Architectural Repertoire of Ligand-Binding Pockets on Protein Surfaces

Pocket science: The structural diversity of ligand-binding pockets of proteins was investigated by using self-organizing pocket frameworks. Pocket frameworks represent the topology of pockets as graphs that were obtained from a growing neural gas approach for pocket topology assignment. Cluster analysis of 623 known ligand binding site topologies suggests an overall limited structural diversity of ligand-accommodating protein cavities.



ChemBioChem
DOI: 10.1002/cbic.200900604



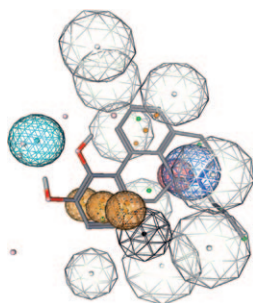
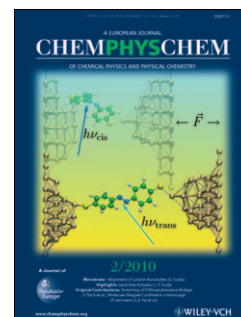
ChemPhysChem
DOI: 10.1002/cphc.200900770

Water Clusters

A. M. Tokmachev,* A. L. Tchougréeff, R. Dronskowski

Hydrogen-Bond Networks in Water Clusters (H₂O)₂₀: An Exhaustive Quantum-Chemical Analysis

H-bond networks: The first exhaustive quantum-chemical calculations of H-bond networks in dodecahedral water clusters (see picture) are described. The millions of configurations considered provide unique statistical data for the energies, spatial and electronic structures of water clusters, thus allowing for insights into the nature of cooperativity in H-bonded systems.



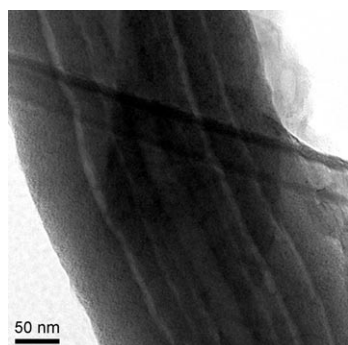
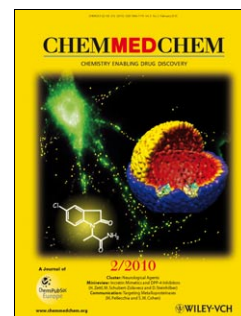
ChemMedChem
DOI: 10.1002/cmdc.200900398

Pharmacophore Modeling

M. Malo, L. Brive, K. Luthman, P. Svensson*

Selective Pharmacophore Models of Dopamine D₁ and D₂ Full Agonists Based on Extended Pharmacophore Features

The reasons for full efficacy and selectivity for dopamine D₁ and D₂ receptor agonists were investigated with pharmacophore models that are based on extended features and excluded volumes. The extended features represent key ligand interaction sites in the receptors. These models reveal useful information for drug design and receptor modeling.



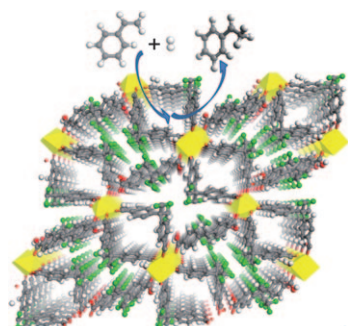
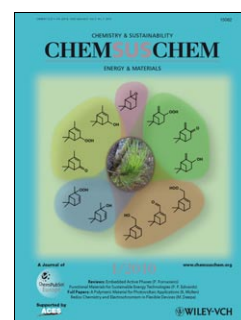
ChemSusChem
DOI: 10.1002/cssc.200900187

Carbon Electrodes

X. Liu, Y.-S. Hu,* J.-O. Müller, R. Schlögl, J. Maier, D. S. Su*

Composites of Molecular-Anchored Graphene and Nanotubes with Multitubular Structure: A New Type of Carbon Electrode

Modified graphene-carbon nanotube composites are synthesized and described. The composites display multitubular co-axial microstructures, consisting of three or more tubes formed along the pristine tube with a homogeneous thickness ranging from 10 to 50 nm.



ChemCatChem
DOI: 10.1002/cctc.200900228

Metal-Organic Frameworks

A. E. Platero Prats, V. A. de la Peña-O'Shea, M. Iglesias, N. Snejko, Á. Monge, E. Gutiérrez-Puebla*

Heterogeneous Catalysis with Alkaline-Earth Metal-Based MOFs: A Green Calcium Catalyst

Cheap thrills: A new metal-organic framework, based on cheap, abundant calcium, with the bent ligand, 4,4'-hexafluoroisopropylidenebis-benzoic acid, serves as a highly efficient heterogeneous catalyst for the hydrogenation of styrene to form ethyl benzene under mild conditions. Complete hydrogenation occurs after 2 h at 373 K without formation of byproducts.



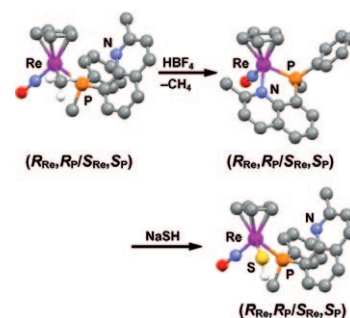


Stereochemistry at Rhenium

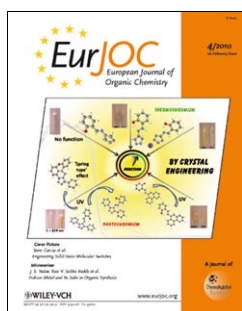
F. Bock, F. Fischer, K. Radacki, W. A. Schenk*

Diastereoselective Protonation, Substitution and Addition Reactions at Pseudotetrahedral Rhenium Complexes

Diastereomerically pure rhenium complexes $[\text{CpRe}(\text{NO})(\text{P}^*-\text{N})(\text{R})]$ have been obtained through a highly diastereoselective intramolecular proton-transfer reaction. The stereochemistry of chelate ring closure/opening was followed by X-ray crystallography for each step. The $\text{Re}-\text{SH}$ complex reacts with aldehydes to give diastereomerically pure thioaldehyde complexes which add nucleophiles with 42–89% *de*.



Eur. J. Inorg. Chem.
DOI: 10.1002/ejic.200901011

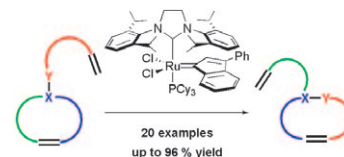


Olefin Metathesis

H. Clavier,* J. Broggi, S. P. Nolan*

Ring-Rearrangement Metathesis (RRM) Mediated by Ruthenium-Indenylidene Complexes

Ruthenium-indenylidene complexes bearing N-heterocyclic carbenes and phosphanes have been investigated and found to promote efficiently the ring rearrangement of several cyclic compounds by alkene metathesis.



Eur. J. Org. Chem.
DOI: 10.1002/ejoc.200901316

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