

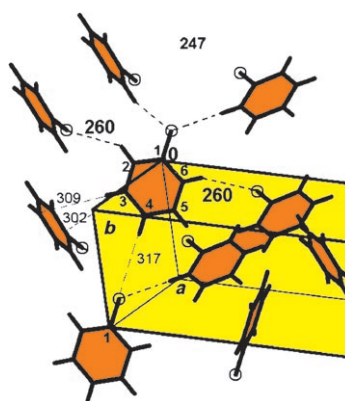
Supramolecular Chemistry

P. Ganguly,* G. R. Desiraju*

Van der Waals and Polar Intermolecular Contact Distances: Quantifying Supramolecular Synthons

Chem. Asian J.

DOI: 10.1002/asia.200700343



Sizing it up: Crystal structures are considered in terms of intermolecular distances, which are determined by environment-dependent atomic sizes. The supramolecular synthons that make up an organic crystal are quantified in terms of the nature of the weak intermolecular interactions (distances shown are in ppm).

Protein Engineering

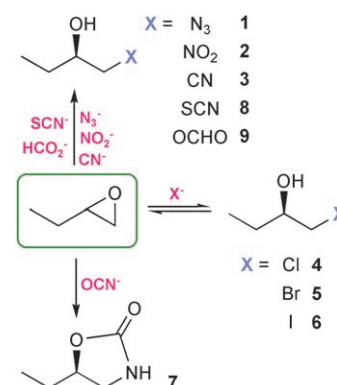
G. Hasnaoui-Dijoux,
M. Majerić Elenkov, J. H. Lutje Spelberg,
B. Hauer, D. B. Janssen*

Catalytic Promiscuity of Halohydrin Dehalogenase and its Application in Enantioselective Epoxide Ring Opening

ChemBioChem

DOI: 10.1002/cbic.200700734

Easy virtue: Halohydrin dehalogenase is a highly promiscuous enzyme that can catalyze enantioselective epoxide ring opening with at least nine different anionic nucleophiles (see scheme). Its capacity to form carbon–nitrogen, carbon–oxygen, carbon–sulfur, and carbon–carbon bonds makes it possible to use this enzyme for the preparation of a range of highly enantioenriched β -substituted alcohols or derivatives thereof, including cyanoalcohols, nitroalcohols, and oxazolidinones.



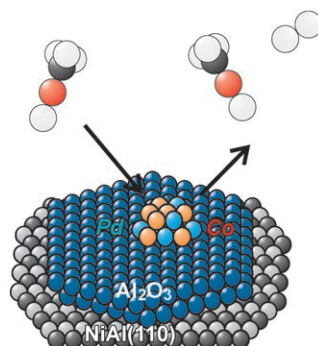
Catalysts

T. Nowitzki, H. Borchert, B. Jürgens,
T. Risse, V. Zielasek, M. Bäumer*

UHV Studies of Methanol Decomposition on Mono- and Bimetallic CoPd Nanoparticles Supported on Thin Alumina Films

ChemPhysChem

DOI: 10.1002/cphc.200700663



One metal or two? Adsorption and reaction studies on well-defined model systems are important to understand the complex surface processes on real catalysts. This fundamental study of the decomposition of methanol on metal clusters (see picture) results in syngas and/or carbon deposits on the particle surfaces depending on their composition.

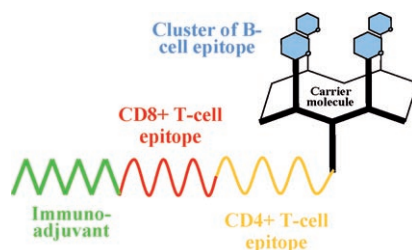
Antitumor Agents

O. Renaudet, L. BenMohamed,
G. Dasgupta, I. Bettahi, P. Dumy*

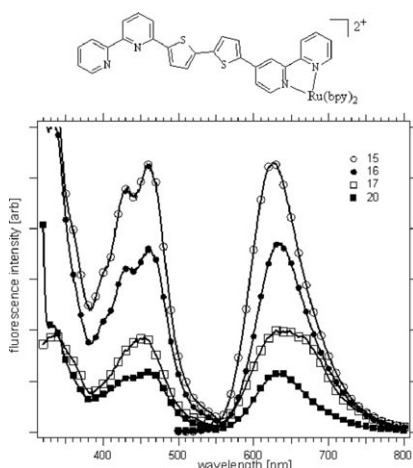
Towards a Self-Adjuvanting Multivalent B and T cell Epitope Containing Synthetic Glycolipopeptide Cancer Vaccine

ChemMedChem

DOI: 10.1002/cmdc.200700315



A new generation of synthetic cancer vaccine: the first self-adjuvanting vaccine prototype combining a cluster of B cell epitope, a CD4 + T helper cell epitope, a CD8 + T cell epitope, and an immuno-adjuvant has been synthesized by a chemo-selective strategy. Vaccination of mice with this molecularly defined construction induces a strong protection against tumors.



A range of mono- and bis(bidentate) 2,2'-bipyridine-capped oligothiophene-bridged Ru^{II} complexes based on the 6-(2-thienyl)-2,2'-bipyridine motif and the 4-(2-thienyl)-2,2'-bipyridine motif have been synthesized, and the luminescence lifetimes and electrochemical potentials have been measured.

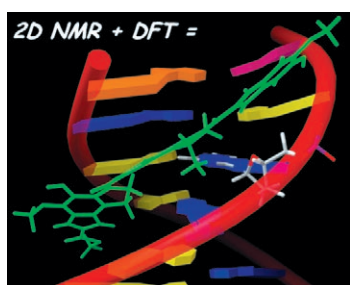
Photophysics

R. O. Steen, L. J. Nurkkala, S. J. Angus-Dunne, C. X. Schmitt, E. C. Constable, M. J. Riley, P. V. Bernhardt, S. J. Dunne*

The Role of Isomeric Effects on the Luminescence Lifetimes and Electrochemistry of Oligothiophenyl-Bridged Dinuclear Tris(2,2'-bipyridine)-ruthenium(II) Complexes

Eur. J. Inorg. Chem.

DOI: 10.1002/ejic.200701118



A hybrid approach based on 2D-NMR spectroscopy and quantum mechanical calculations of ¹H chemical shifts at the DFT/MPW1PW91 level was used for the characterization of the covalent complex formed by (+)-yatakemycin and d(GAC-TAATTGAC)-(GTCAATTAGTC), showing that calculation of NMR parameters can be a useful tool for the structural characterization of ligand–receptor interactions.

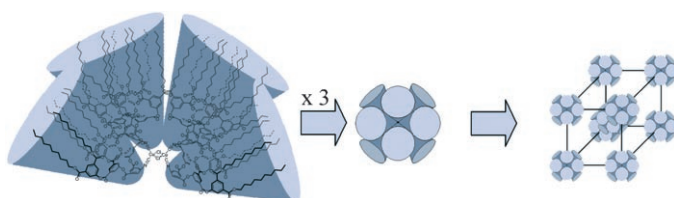
Ligand–Receptor Interactions

S. Di Micco, D. L. Boger, R. Riccio, G. Bifulco*

Structural Features of the (+)-Yatakemycin/d(GACTAATTGAC)-(GTCAATTAGTC) Complex – Quantum Mechanical Calculation of NMR Parameters as a Tool for the Characterization of Ligand/DNA Interactions

Eur. J. Org. Chem.

DOI: 10.1002/ejoc.200701212



Branching out! Stable metallodendrimers made from monodendrons with an isocyanide group in the focal point have been prepared. Although the molecules of the metallodendrimers prepared are structurally very different, consisting of one, two,

or four monodendrons, the structures of the mesophases are similar and consist of the packing of micellar aggregates in a three-dimensional cubic *Im3m* lattice (see scheme).

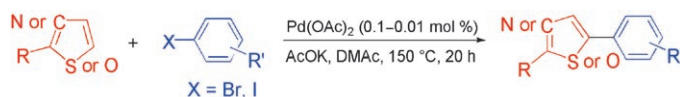
Metallodendrimers

S. Coco,* C. Cordovilla, B. Donnio, P. Espinet,* M. J. García-Casas, D. Guillon

Self-Organization of Dendritic Supermolecules, Based on Isocyanide–Gold(I), –Copper(I), –Palladium(II), and –Platinum(II) Complexes, into Micellar Cubic Mesophases

Chem. Eur. J.

DOI: 10.1002/chem.200800128



How low can Pd go? The direct arylation of heteroaryl compounds under very low loadings of Pd(OAc)₂ as catalyst and in the absence of any added ligand proceeds in high yield. Turnover numbers

up to 10 000 are observed for the coupling of activated aryl bromides with thiazole, thiophene or furan derivatives (see scheme; DMAc = N,N-dimethylacetamide).

Homogeneous Catalysis

F. Požgan, J. Roger, H. Doucet*

Ligand-Free Palladium-Catalysed Direct Arylation of Heteroaromatics Using Low Catalyst Loadings

ChemSusChem

DOI: 10.1002/cssc.200700166