Spotlights ...

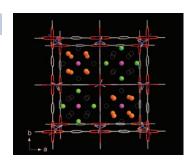


Gas Storage

H. Kim, D. G. Samsonenko, S. Das, G.-H. Kim, H.-S. Lee, D. N. Dybtsev, E. A. Berdonosova, K. Kim*

Methane Sorption and Structural Characterization of the Sorption Sites in Zn₂(bdc)₂(dabco) by Single Crystal X-ray Crystallography

Store it away: Methane adsorption isotherms of Zn₂(bdc)₂(dabco) (1) are measured up to a pressure of 35 bar. X-ray structure analysis of methane-adsorbed 1 at 90 K reveals that methane molecules occupy three independent sorption sites A, B, and C while interacting with the framework as well as each other through van der Waals interactions.



Chem. Asian I.

DOI: 10.1002/asia.200900020



Peptidomimetics

A. Grässlin, C. Amoreira, K. K. Baldridge, * J. A. Robinson *

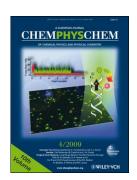
Thermodynamic and Computational Studies on the Binding of p53-Derived Peptides and Peptidomimetic Inhibitors to HDM2

Helix power: The binding interactions of linear and constrained β -hair-pin-shaped peptides with HDM2 were compared by using experimental and theoretical methods. The entropic advantages enjoyed by the constrained peptides were found to be largely offset by reduced enthalpic contributions to binding of the cyclic mimetics. Formation of hydrogen bonds upon helix folding could contribute significantly to the enhanced enthalpy observed in binding of the linear peptides.



ChemBioChem

DOI: 10.1002/cbic.200900008

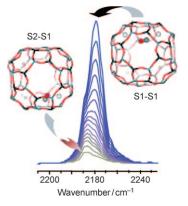


Zeolites

A. Pulido, P. Nachtigall, M. Rodríguez Delgado, C. Otero Areán*

Computational and Variable-Temperature Infrared Spectroscopic Studies on Carbon Monoxide Adsorption on Zeolite Ca-A

Bridged Ca²⁺···CO···Ca²⁺ complexes are formed on dual-cation sites, constituted by a pair of nearby Ca²⁺ cations, when CO is adsorbed on zeolite Ca-A. Two types of such species can be formed, designated S2–S1 and S1–S1 (see picture). Ca²⁺···CO monocarbonyl species are also identified, and at a relatively high CO equilibrium pressure, dicarbonyl complexes can also form.



Chem Phys Chem

DOI: 10.1002/cphc.200800843

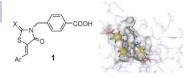


Drug Design

R. Maccari,* R. Ottanà, R. Ciurleo, P. Paoli, G. Manao, G. Camici, C. Laggner, T. Langer

Structure-Based Optimization of Benzoic Acids as Inhibitors of Protein Tyrosine Phosphatase 1B and Low Molecular Weight Protein Tyrosine Phosphatase

We have optimized previously discovered benzoic acids 1, which are active as inhibitors of PTP1B and LMW-PTP, two protein tyrosine phosphatases that have emerged as attractive targets for the development of novel therapeutic agents for the treatment of diabetes, obesity, and cancer. Our efforts led to the identification of new and more potent analogues with appreciable selectivity toward human PTP1B and the IF1 isoform of human LMW-PTP.



ChemMedChem

DOI: 10.1002/cmdc.200800427

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+ Cu₂(CH₃COO)₄(H₂O)₂ → p-PyV· Cu₂(CH₃COO)₄(ρ-PyV·)₂

Eur. J. Inorg. Chem. DOI: 10.1002/ejic.200900004

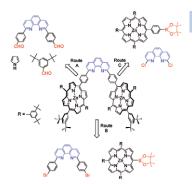
Copper-Verdazyl Complex

A. V. Yakovenko, S. V. Kolotilov, O. Cador, S. Golhen, L. Ouahab,* V. V. Pavlishchuk*

Structure, Spectral and Magnetic Properties of 3-(p-Pyridyl)-1,5-diphenylverdazyl (p-PyV) and the Binuclear Copper(II) Radical Complex [Cu₂(OCOCH₃)₄(p-PyV)₂]

Pyridyl-substituted verdazyl (p-PyV) and the binuclear copper complex $[Cu_2(OCOCH_3)_4(p$ -PyV) $_2]$ are synthesized and structurally characterized. Their magnetic properties are studied by ESR spectroscopy and by measuring their temperature-dependent magnetic susceptibility.





Eur. J. Org. Chem.

DOI: 10.1002/ejoc.200900149

Gable Bis(porphyrin)s

M. Beyler, C. Beemelmanns, V. Heitz,* J.-P. Sauvage

Various Synthetic Routes to a Gable-Like Bis (porphyrin) Constructed on a 1,10-Phenanthroline Chelate

The synthesis of a gable-like bis(porphyrin) constructed on a 1,10-phenanthroline chelate by three different approaches is described.



Halogen–Metal Exchange Reactions

Chem. Eur. J.

DOI: 10.1002/chem.200802393

Halogen-Zinc Exchange

S. Nakamura,* C.-Y. Liu, A. Muranaka, M. Uchiyama*

Theoretical Study on the Halogen–Zinc Exchange Reaction by Using Organozincate Compounds

Zincate it! The mechanism of the halogen–zinc exchange reaction with organozincate compounds has been studied by using density functional theory to elucidate the effects of changing the halogen species, the alkyl ligand on zinc, and the substrate nature (see figure).





ChemSusChem

DOI: 10.1002/cssc.200800260

Catalysis

T. Ishida,* M. Haruta

N-Formylation of Amines via the Aerobic Oxidation of Methanol over Supported Gold Nanoparticles

Dress code: formyl. Gold nanoparticles supported on NiO catalyze the one-pot *N*-formylation of amines with methanol and molecular oxygen to produce formamide at a selectivity of 90%. This process generates methyl formate in situ, followed by reaction with amines.





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