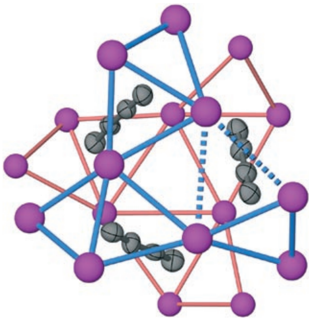
Spotlights ...

Supramolecular Chemistry

L. Zhao, M. Du, T. C. W. Mak*

Silver(I) Double and Multiple Salts Containing the 1,3-Butadiynediide Dianion: Coordination Diversity and Assembly with the Supramolecular Synthon $Ag_4{\subset}C{\equiv}C{-}C{\equiv}C{\supset}Ag_4$

Chem. Asian J.
DOI: **10.1002/asia.200700193**



Silver rings and baskets: The $[Ag_4C_4Ag_4]$ aggregate adopts diverse configurations in a series of 13 silver(I) complexes with a consistent μ_8 bonding mode for C_4^{2-}. The configurations can be tuned by varying the ancillary anionic ligands. The largest silver–ethynide aggregate identified to date, $(C_4)_3@Ag_{18}$ (shown), occurs in $3\,Ag_2C_4\cdot 12\,AgC_2F_5CO_2\cdot 5\,[(BnMe_3N)C_2F_5CO_2]\cdot 4\,H_2O$ (Bn = benzyl).

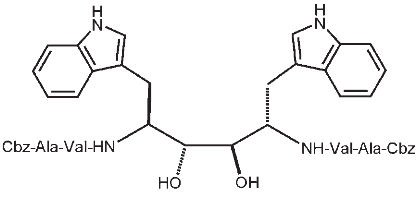
Protease Inhibitors

Y.-M. Shao, W.-B. Yang, H.-P. Peng, M.-F. Hsu, K.-C. Tsai, T.-H. Kuo, A. H.-J. Wang, P.-H. Liang C.-H. Lin, A.-S. Yang* C.-H. Wong*

Structure-Based Design and Synthesis of Highly Potent SARS-CoV 3CL Protease Inhibitors

ChemBioChem
DOI: **10.1002/cbic.200700254**

In a successful example of lead optimization by computer modeling prediction, computational technology was used to optimize a lead inhibitor (TL-3) of the SARS-CoV 3CL protease. A novel C_2-symmetric diol (**1**) was then designed and synthesized, and displayed higher affinity than the original lead compound by one order of magnitude in its inhibition constant (0.6→0.073 μM). We believe that this approach has provided a platform for further lead optimization.



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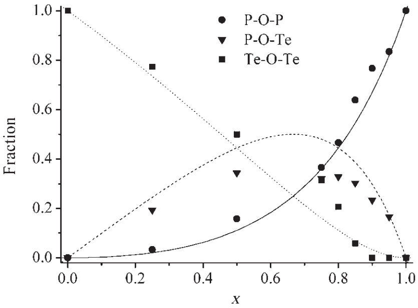
Solid-State NMR Spectroscopy

M. T. Rinke, L. Zhang, H. Eckert*

Structural Integration of Tellurium Oxide into Mixed-Network-Former Glasses: Connectivity Distribution in the System $NaPO_3$–TeO_2

ChemPhysChem
DOI: **10.1002/cphc.200700358**

Sodium phosphate tellurite glasses prepared and structurally characterized by XP and NMR spectroscopies, show no new structural units and no sharing of the network modifier. The resulting chemical segregation leads to a nonrandom sodium distribution. The picture shows the fraction of different linkages in a $(NaPO_3)_x(TeO_2)_{1-x}$ glass.

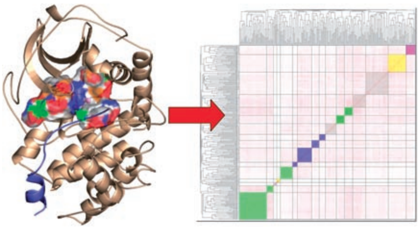


Similarity Analysis

D. Kuhn, N. Weskamp, E. Hüllermeier, G. Klebe*

Functional Classification of Protein Kinase Binding Sites Using Cavbase

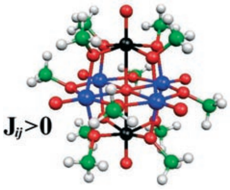
ChemMedChem
DOI: **10.1002/cmdc.200700075**



A diverse set of 258 kinases has been analyzed and clustered based on the exposed physicochemical properties of their ATP binding sites using Cavbase. The resulting clustering provides a relevant grouping of the kinases. Furthermore, pairs of kinases are identified that show unexpected similarities in their binding sites independent of their distance in sequence space.

Ferroexchange in Polyoxovanadates

DFT calculations suggest that the V^{IV}/V^{V} mixed-valence alkoxo-polyoxovanadate $[4V^{IV} + 2V^{V}]$ is valence-trapped and characterized by ferromagnetic interactions between vanadium(IV) centers.

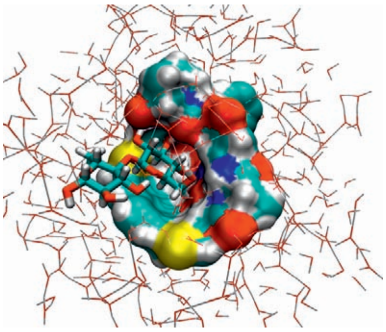


E. M. Zueva,* S. A. Borshch,*
M. M. Petrova, H. Chermette,
A. M. Kuznetsov

Ferromagnetic Coupling in a Mixed-Valence Hexavanadate Core: Quantum-Chemical Forecast

Eur. J. Inorg. Chem.
DOI: **10.1002/ejic.200700421**

Organic Peptide Receptors



An artificial, water-soluble and bicyclic peptide receptor for carbohydrates was constructed and the binding of disaccharides was studied in water by using NMR spectroscopy and mass spectrometry. The receptor contains an aromatic bridge fused to a cyclic dodecapeptide to form a cage-like receptor.

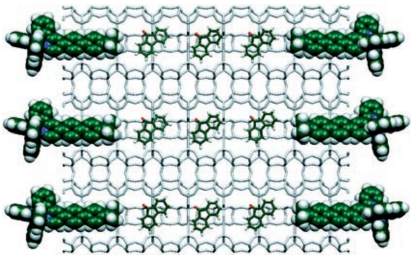
T. Reenberg, N. Nyberg, J. Ø. Duus,
J. L. J. van Dongen, M. Meldal*

Specific Recognition of Disaccharides in Water by an Artificial Bicyclic Carbohydrate Receptor

Eur. J. Org. Chem.
DOI: **10.1002/ejoc.200700518**

Zeolites

Superacidic nanochannels: Zeolite L crystals that have been partially exchanged with protons are super acids. The diagram shows protonation of a molecule dye in the ground state and in the electronically excited state (see graphic). The proton activity inside the channels of zeolite L has been studied.



R. Q. Albuquerque, G. Calzaferri*

Proton Activity Inside the Channels of Zeolite L

Chem. Eur. J.
DOI: **10.1002/chem.200700569**

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