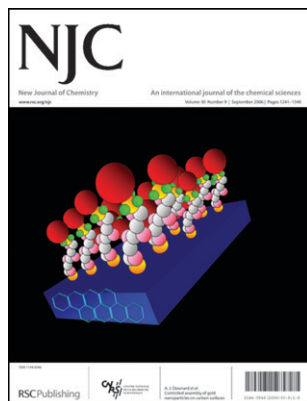


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ISSN 1144-0546 CODEN NJCHES 30(9) 1241-1348 (2006)



Cover

See Alison J. Downard *et al.*, p. 1283. Citrate-capped gold nanoparticles assemble on amine tethers, electrochemically grafted to a carbon film. Image reproduced by permission of Alison J. Downard, Emelyn S. Q. Tan and Samuel S. C. Yu, *New J. Chem.*, 2006, **30**, 1283.

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C65

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Chemical Science

September 2006/Volume 3/Issue 9

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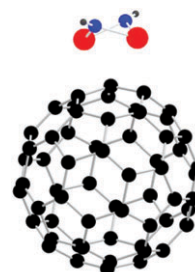
PERSPECTIVE

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Dinitrogen fixation and activation by Ti and Zr atoms, clusters and complexes

Navaratnarajah Kuganathan, Jennifer C. Green and Hans-Jörg Himmel*

New discoveries from the "worlds" of solution chemistry and matrix isolation shed light on dinitrogen activation by the early transition metal elements Ti and Zr and their potential applications.



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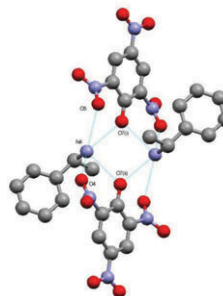


1263

Experimental evidence for the homochiral aggregation of ammonium salts in solution

Ana M. Costero,* Manuel Colera, Pablo Gaviña, Salvador Gil and Luis E. Ochando

NMR and X-ray evidence for the homochiral aggregation of chiral ammonium picrates from racemic solutions is presented.



PAPERS

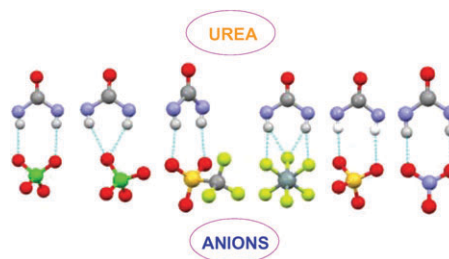


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Exploring conformationally flexible hydrogen-bond-functionalized ligand and counter anions in metal-organic frameworks of Cu(II)

D. Krishna Kumar, Amitava Das* and Parthasarathi Dastidar*

Structures of Cu(II) MOFs show that the counter anions are recognized by the urea functionality of the ligand backbone and contribute significantly in shaping the resultant frameworks and their stability.

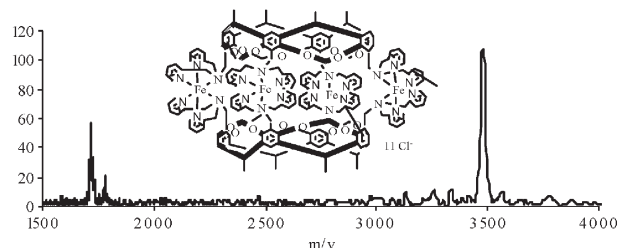


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Sonic spray ionization mass spectrometry: a powerful tool used to characterize fragile metal-assembled cages

Joseph S. Gardner, Roger G. Harrison,* John D. Lamb* and David V. Dearden*

High molecular weight ions are observed for metal-assembled cages by sonic spray ionization mass spectrometry.

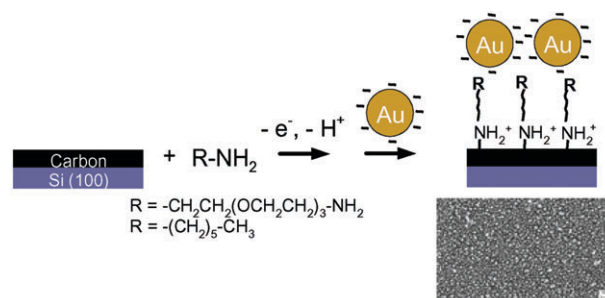


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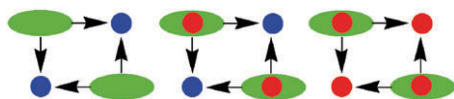
Controlled assembly of gold nanoparticles on carbon surfaces

Alison J. Downard,* Emelyn S. Q. Tan and Samuel S. C. Yu

Amine tethers are electrochemically grafted to carbon surfaces giving a covalently-attached film for electrostatic assembly of citrate-capped nanoparticles. Control of the grafting conditions is a simple method for tuning the nanoparticle assembly.



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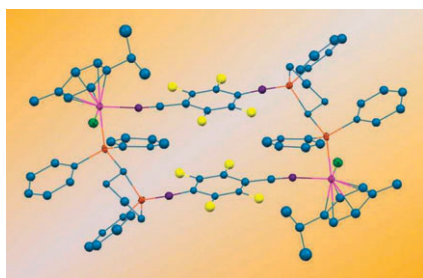


Porphyrin based metallamacrocycles

Emmanuel Deiters, Véronique Bulach* and Mir Wais Hosseini*

A porphyrin derivative bearing two peripheral pyridine units and its metallated analogue leads in the presence of metal halides to homo- and hetero-nuclear [2 + 2] metallamacrocycles.

1295

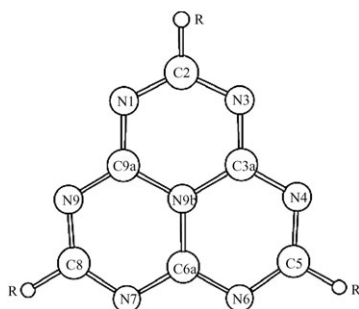


Imination reactions of free and coordinated 2-diphenylphosphino-1-phenyl-phospholane: Access to regioisomeric ruthenium(II) complexes containing novel iminophosphorane–phosphine ligands

A. E. Díaz-Álvarez, P. Crochet,* M. Zablocka,* V. Cadierno, C. Duhayon, J. Gimeno and J.-P. Majoral*

Neutral or cationic mono- and dinuclear (η^6 -arene)–ruthenium(II) complexes incorporating regioisomeric iminophosphorane–phosphine ligands were prepared from an unsymmetrical phosphino–phospholane ligand.

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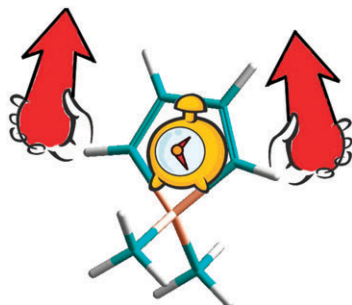


Absorption spectra of tri-*s*-triazines: time dependent density functional theory calculations

Wenxu Zheng, Ning-Bew Wong,* Wai-Kee Li and Anmin Tian*

The absorption spectra of tri-*s*-triazines in gas phase and in ethanol solvent have been calculated by using time-dependent density functional theory (TDDFT). The computed results show a good agreement with the available experimental data.

1319



Towards a better understanding of photo-excited spin alignment processes using silole diradicals

Nans Roques, Philippe Gerbier,* Yoshio Teki,* Sylvie Choua, Petra Lesniaková, Jean-Pascal Sutter, Philippe Guionneau and Christian Guérin

Despite the presence of both an appropriate topology for the molecule and well-tried iminonitroxide radicals, siloles did not allow observation of any photo-excited high-spin states within the timescale of the TRESR measurement.

PAPERS

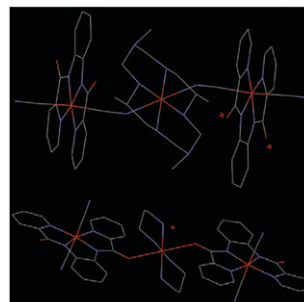


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Heterometallic trinuclear $\text{Cu}^{\text{II}}\text{M}^{\text{III}}_2$ ($\text{M} = \text{Fe}$ or Cr) complexes with novel bridges and unusual magnetic properties

Bing Zhang, Zhong-Hai Ni, Ai-Li Cui and Hui-Zhong Kou*

The magnetic properties of trinuclear bimetallic complexes comprised of four-coordinate $\text{Cu}(\text{II})$ complexes and $[\text{M}(\text{bpb})(\text{CN})_2]^-$ have been investigated.

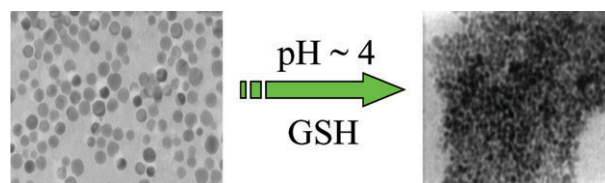


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Dipole–dipole plasmon interactions in self-assembly of gold organosol induced by glutathione

Soumen Basu, Sudipa Panigrahi, Snigdhamayee Praharaj, Sujit Kumar Ghosh, Surojit Pande, Subhra Jana and Tarasankar Pal*

A controlled method of aggregation of gold nanoparticles in organic solvents has been achieved under controlled pH conditions with different concentrations of the molecular linker glutathione to study the plasmon–plasmon interactions amongst the gold nanoparticles.

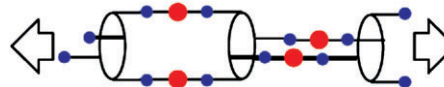


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Molecular tectonics: on the formation of tubular coordination networks

Guillaume Laugel, Ernest Graf, Mir Wais Hosseini,* Jean-Marc Planeix and Nathalie Kyritsakas

A macrocyclic tecton bearing four pyridine units occupying the apices of a tetrahedron leads in the presence of silver cation to the formation of tubular metalloorganic architecture.



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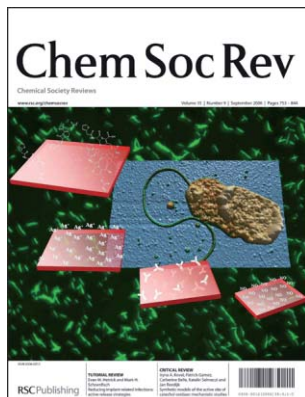
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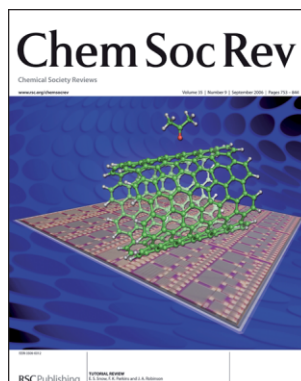
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See Evan M. Hetrick and Mark H. Schoenfisch, page 780. Bacterial adhesion and active release strategies to combat implant-related infections. Image reproduced by permission of Evan M. Hetrick and Mark H. Schoenfisch, *Chem. Soc. Rev.*, 2006, 35, 780.



Inside cover

See E. S. Snow, F. K. Perkins and J. A. Robinson, page 790. An expanded view (covering 7 orders of magnitude in scale) of a wafer of chemical sensors that use networks of carbon nanotubes as the active sensor material. Image reproduced by permission of E. S. Snow, F. K. Perkins and J. A. Robinson, *Chem. Soc. Rev.*, 2006, 35, 790.

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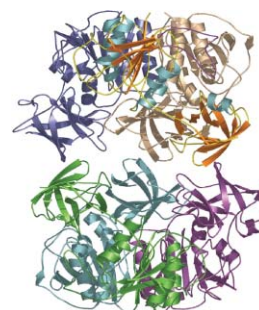
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Inferring the chemical mechanism from structures of enzymes

James H. Naismith

Structural studies of enzymes can help unravel fascinating chemical mechanisms.

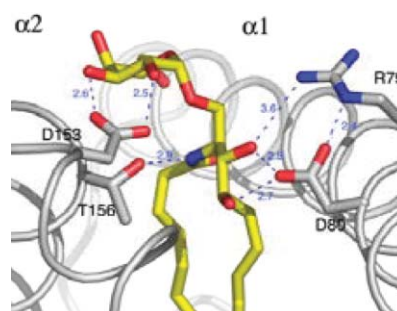


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Glycolipids for natural killer T cells

Paul B. Savage,* Luc Teyton and Albert Bendelac

Carbohydrate and lipid recognition combine to select for specific glycolipids that stimulate strong immune responses from natural killer T cells.

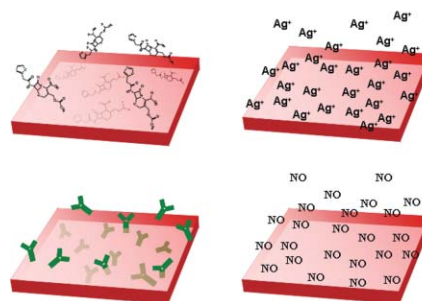


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Reducing implant-related infections: active release strategies

Evan M. Hetrick and Mark H. Schoenfisch*

Polymeric coatings that actively release antibacterial mediators have been designed to reduce implant-associated infection. Current active release strategies include the use of antibiotics, silver ion, antibodies, and nitric oxide.

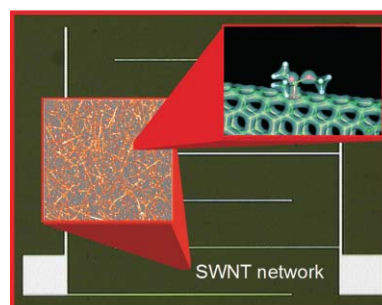


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Chemical vapor detection using single-walled carbon nanotubes

E. S. Snow, F. K. Perkins and J. A. Robinson

Transitioning carbon nanotubes from laboratory curiosity to chemical sensor applications.

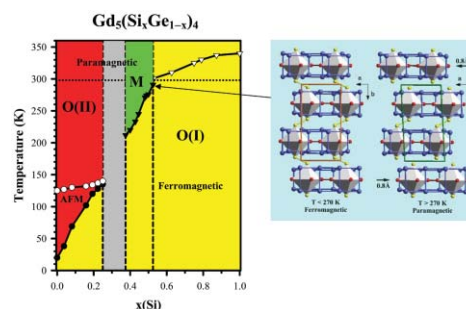


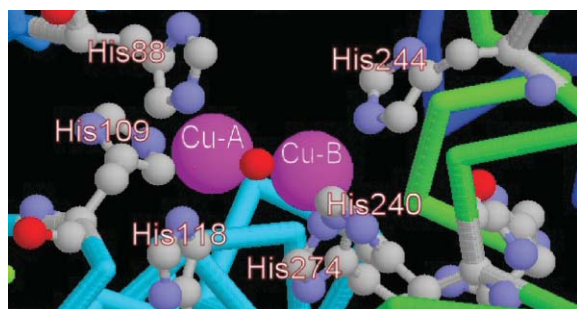
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Complex rare-earth tetrelides, $\text{RE}_5(\text{Si}_x\text{Ge}_{1-x})_4$: New materials for magnetic refrigeration and a superb playground for solid state chemistry

Gordon J. Miller

Near-room temperature magnetic refrigeration can become viable through fundamental chemical and physical investigations of the rare-earth series, $\text{RE}_5(\text{Si}_x\text{Ge}_{1-x})_4$.





Synthetic models of the active site of catechol oxidase: mechanistic studies

Iryna A. Koval, Patrick Gamez, Catherine Belle, Katalin Selmecezi and Jan Reedijk*

Catechol oxidase is a type-3 copper enzyme responsible for the production of melanin, a dark pigment thought to protect a damaged tissue from pathogens. This *critical review* (citing 114 references) summarizes the past two decades of research on the active site of catechol oxidase, and extensively discusses studies on model compounds of the enzyme in order to disclose the mechanism of the enzymatic conversion.

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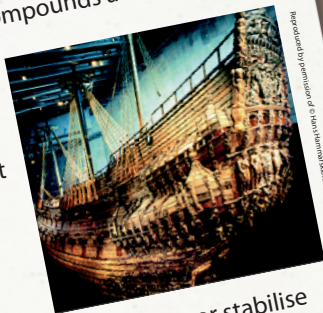
It's our largest body organ, covering about two square metres and weighing around 5 kilograms. This review discusses how a deeper understanding of skin biochemistry holds the key to the development of future therapies for skin conditions such as contact dermatitis and skin cancer.



Biochemistry of human skin—our brain on the outside,
D. J. Tobin, *Chem. Soc. Rev.*, 2006, **35**, 52

Preserving the past

Oxidation of sulfur compounds accumulated in the wood of historical shipwrecks may cause severe acidity in the moist wood, potentially accelerating degradation of recovered archaeological artefacts. Will methods to remove or stabilise sulfur compounds in the wood save the day?



Sulfur and iron in shipwrecks cause conservation concerns, Y. Fors and M. Sandström, *Chem. Soc. Rev.*, 2006, **35**, 399

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