

In this issue...

The direct synthesis of ordered mesoporous silica containing fluorinated chains using fluorinated surfactants. See Catherine Reyé *et al.*, page 538.



Cover

The front cover shows the Photoactive Yellow Protein (PYP) active site and its laser-induced picosecond spectroscopy. PYP is the photoreceptor responsible for the photoavoidance response of the purple bacterium *Halorhodospira halophila* to blue light. The photon absorption triggers an intracellular reaction chain that leads to flagella motion and escape. Image reproduced by permission of Pascale Chagenet-Barret, Agathe Espagne, Pascal Plaza, K. J. Hellingwerf and Monique M. Martin from *New J. Chem.*, 2005, **29**, 527.

CHEMICAL SCIENCE

C25

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Chemical Science

April 2005/Volume 2/Issue 4

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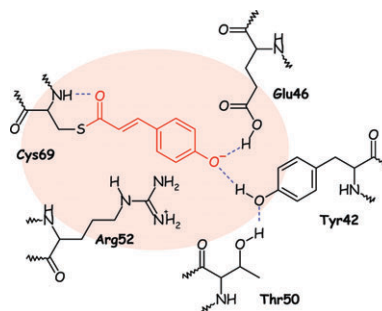
PERSPECTIVE

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Investigations of the primary events in a bacterial photoreceptor for photomotility: photoactive yellow protein (PYP)

Pascale Chagenet-Barret,* Agathe Espagne, Pascal Plaza, K. J. Hellingwerf and Monique M. Martin

We review the comparative study of native PYP and several chromophore analogues in solution in order to try to further clarify the early steps of the photocycle.



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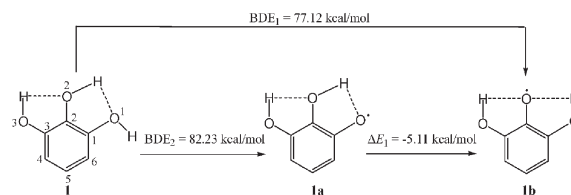
LETTER

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A CCSD estimation of the O–H bond dissociation enthalpies of pyrogallol

Hong-Fang Ji and Hong-Yu Zhang*

The O–H bond dissociation enthalpy of pyrogallol was estimated by means of CCSD calculations to be 10.48 kcal mol⁻¹ lower than that of phenol, which is in excellent agreement with the experimental value determined by time-resolved photoacoustic calorimetry.



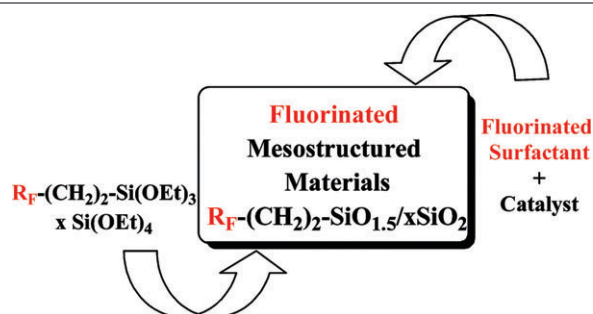
PAPERS

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Direct syntheses using a fluorinated surfactant of silicas containing organofluorinated groups

Olivier Porcherie, Yannick Guari and Catherine Reyé*

Mesostructured fluorinated silica materials, $R_F(CH_2)_2SiO_{1.5} \cdot xSiO_2$ [$R_F = CF_3(CF_2)_5$ or CF_3], were prepared using the fluorinated surfactants $C_8F_{17}(CH_2)_2NMe_3^+ I^- \cdot 2KI$ or $C_8F_{17}(CH_2)_2NH_2$ as templating agents.

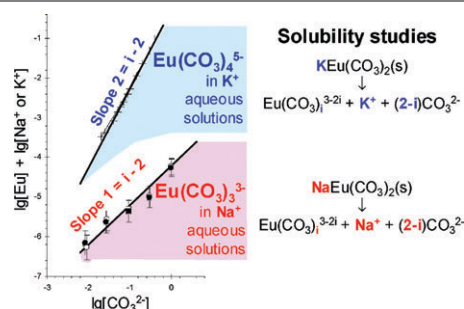


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$Eu(CO_3)_3^{3-}$ and the limiting carbonate complexes of other M^{3+} f-elements in aqueous solutions: a solubility and TRFS study

Thomas Vercoeur,* Pierre Vitorge,* Nicolas Trigoulet, Eric Giffaut and Christophe Moulin

$Eu(CO_3)_3^{3-}$ is the limiting $Eu(III)$ complex in concentrated Na_2CO_3 aqueous solutions, similar to $Nd(III)$ and $Am(III)$, while $Ln(CO_3)_4^{5-}$ preferentially forms with $Ce(III)$ and with the heavier $Ln(III)$ in concentrated K_2CO_3 solutions.

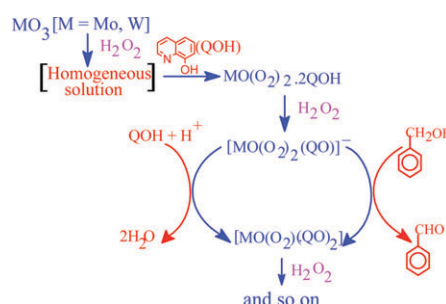


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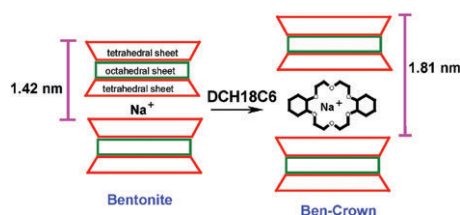
Oxoperoxo molybdenum(vi) and tungsten(vi) and oxodiperoxo molybdate(vi) and tungstate(vi) complexes with 8-quinolinol: synthesis, structure and catalytic activity

Swarup K. Maiti, Surajit Banerjee, Alok K. Mukherjee, K. M. Abdul Malik and Ramgopal Bhattacharyya*

Four new Mo and W oxo(di)peroxo species behave as efficient catalysts in the peroxidic oxidation of alcohols, sulfides and amines.



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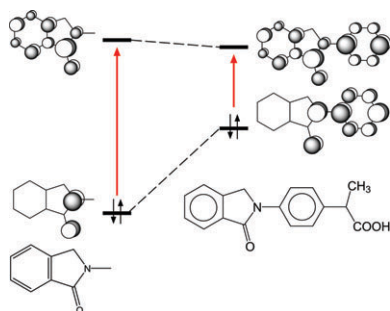


Unusual extraction behaviour of crown ether when intercalated in bentonite

M. V. Sivaiah, K. A. Venkatesan, P. Sasidhar,*
R. M. Krishna and G. S. Murthy

Dicyclohexano-18-crown-6 intercalated into bentonite extracts cesium and strontium with unusually high efficiency from nitric acid, especially at low acid concentrations.

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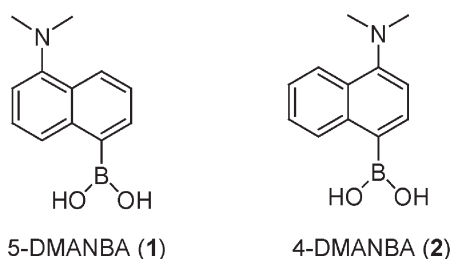


Absorption and solvatochromic properties of 2-methylisindolin-1-one and related compounds: interplay between theory and experiments

Fabien Gutierrez, Jérôme Trzcionka, Rodolphe Deloncle,
Romuald Poteau and Nadia Chouini-Lalanne

The electronic structure of DNA photosensitizers having an isindolinone chromophore is correlated with their absorbance spectra.

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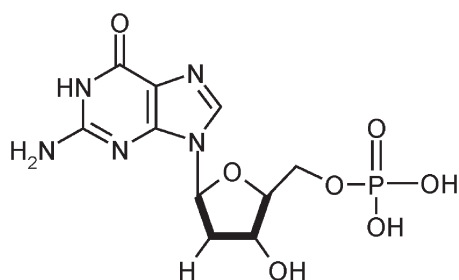


Naphthalene-based water-soluble fluorescent boronic acid isomers suitable for ratiometric and off-on sensing of saccharides at physiological pH

Xingming Gao, Yanling Zhang and Binghe Wang*

Two water-soluble naphthalene-based fluorescent boronic acid isomers are synthesized and exhibit different fluorescence properties: 5-DMANBA is a ratiometric saccharide sensor, while 4-DMANBA is an off-on fluorescent saccharide sensor.

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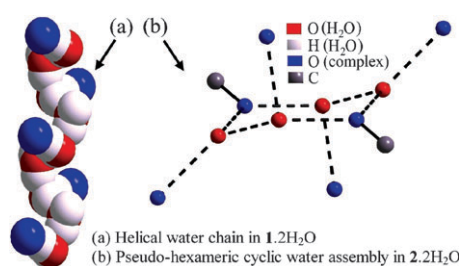


Investigations of electron-transfer reactions and the redox mechanism of 2'-deoxyguanosine-5'-monophosphate using electrochemical techniques

Rajendra N. Goyal,* Sham M. Sondhi and
Anand M. Lahoti

The electrooxidation of 2'-deoxyguanosine-5'-monophosphate forms a variety of products that arise from a series of redox and chemical reactions.

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Effect of carboxylate spacers on the supramolecular self-assembly of dicopper(II) Schiff base complexes stabilizing water assemblies of different conformations

Arindam Mukherjee, Manas K. Saha, Munirathinam
Nethaji and Akhil R. Chakravarty*

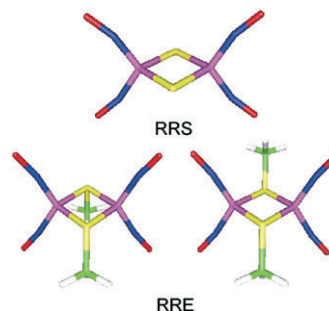
Supramolecular structures of three dicopper(II) complexes containing a pentadentate Schiff base and carboxylate HO-*p*-C₆H₄-X-CO₂⁻ ligands show the formation of water aggregates of different conformations.

604

Structure and UV-Vis spectroscopy of the iron-sulfur dinuclear nitrosyl complexes $[\text{Fe}_2\text{S}_2(\text{NO})_4]^{2-}$ and $[\text{Fe}_2(\text{SR})_2(\text{NO})_4]$

Maria Jaworska* and Zofia Stasicka

The opposing charges on the sulfur atoms in Roussin's red salt dianion (RRS) and Roussin's red diester (RRE) explain the different reactivity of these two species, favouring electrophilic attack for RRS and nucleophilic attack for RRE.

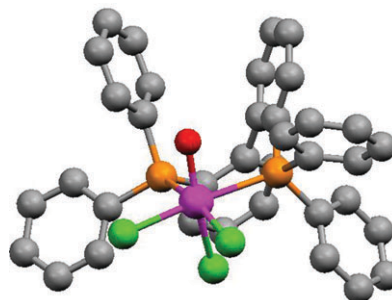


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Synthesis, characterization and structural investigation of new rhenium-oxo complexes containing bidentate phosphine ligands: an exploration of chirality and conformation in chelate rings of small and large bite angle ligands

Maria L. Parr,* Carmen Perez-Acosta and J. W. Faller

The synthesis and characterization of five new rhenium-oxo complexes incorporating bidentate organophosphorus ligands with various bite angles is reported.

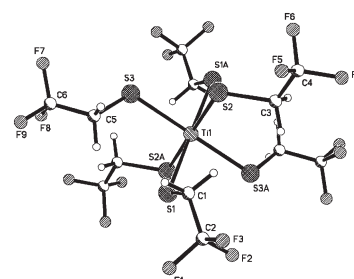


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Reactivity of tetrakisdimethylamido-titanium(IV) and -zirconium(IV) with thiols

Claire J. Carmalt,* Emily S. Peters, Ivan P. Parkin and Derek A. Tocher

Group(IVb) thiolates, $[\text{Me}_2\text{NH}_2]_2[\text{Ti}(\text{SCH}_2\text{CF}_3)_6]$, $[\text{Me}_2\text{NH}_2][\text{Zr}_2(\mu\text{-SBu}^t)_3(\text{SBu}^t)_6]$ and $[\text{Zr}(\text{SC}_5\text{H}_4\text{N})_4]$ have been synthesised from the reaction of $[\text{M}(\text{NMe}_2)_4]$ ($\text{M} = \text{Ti}, \text{Zr}$) with thiols. Low pressure CVD of $[\text{Me}_2\text{NH}_2]_2[\text{Ti}(\text{SCH}_2\text{CF}_3)_6]$ produced TiS_2 films on glass substrates at 550°C .

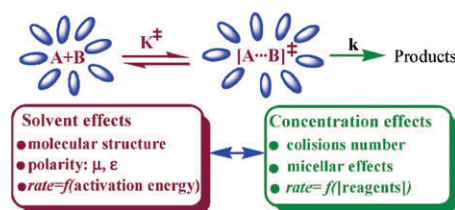


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Solvent effects versus concentration effects in determining rates of base-catalyzed keto-enol tautomerization

Emilia Iglesias*

In homogeneous solvents, solvent effects are due to changes in solvent polarity or in the molecular structure of solvent molecules; in microheterogeneous solvents, such as micellar solutions, concentration effects cannot be avoided.

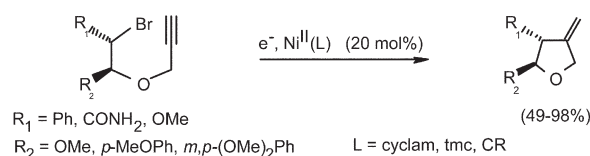


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Electrochemical intramolecular cyclisation of propargyl bromoethers catalysed by nickel complexes

Elisabet Duñach, Ana Paula Esteves, Maria J. Medeiros* and Sandra Olivero

Electrochemical radical-type cyclisations of propargyl derivatives catalysed by Ni^{II} complexes at room temperature lead to good yields of 5-membered ring ether products.




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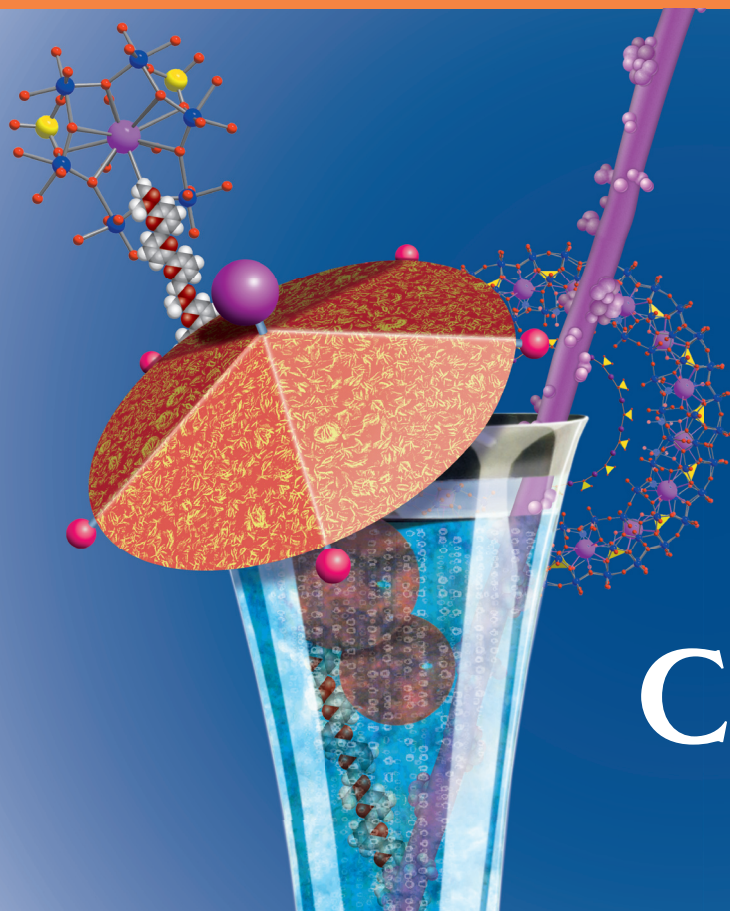
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