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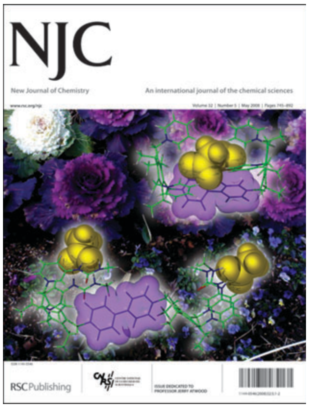
ISSN 1144–0546 CODEN NJCHES 32(5) 745–892 (2008)



Cover
See Steed *et al.*, pp. 786–789. The cover image shows two viologen-based colourimetric anion sensors that respond to different amounts of anion depending on internal competition within the molecules. They are superimposed on an image of flowers taken in Tachikawa, Japan. The colours reflect the colour changes undergone by the anion sensors. Image reproduced with permission from Jonathan W. Steed *et al.* from *New J. Chem.*, 2008, **32**, 786.

Inside Cover
See Robinson *et al.*, pp. 774–776. The cover displays the structure of a molecule containing the first unsupported group 13–hafnium bonds (pink orbs = group 13 elements; blue orb = hafnium). Two identical group 13 metals are bonded to the central hafnium atom resulting in a "V-shaped" core architecture. Image reproduced with permission from Gregory H. Robinson *et al.* from *New J. Chem.*, 2008, **32**, 774.

CHEMICAL SCIENCE

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Drawing together the research highlights and news from all RSC publications, *Chemical Science* provides a 'snapshot' of the latest developments across the chemical sciences, showcasing newsworthy articles and significant scientific advances.

Chemical Science

May 2008/Volume 5/Issue 5

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EDITORIAL

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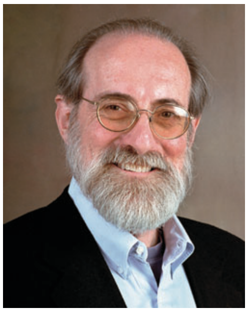
Introduction to the special issue in honour of Jerry Atwood

A collection of papers dedicated to Jerry Atwood on the occasion of his 65th birthday.



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PERSPECTIVE

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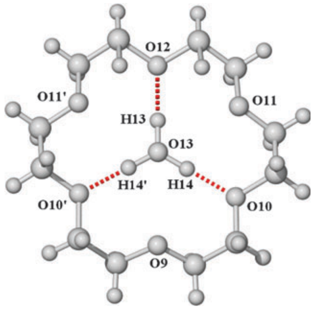
Crown ethers as stabilising ligands for oxonium ions

Peter C. Junk

Crown ethers can be used to isolate oxonium ions ($H^+ \cdot (H_2O)_n$ (n = 1, 2, 3, 4)). The structure and oligonuclearity of the oxonium ion depends on the hydrogen bonding acceptor properties of the immediate environment.



LETTERS

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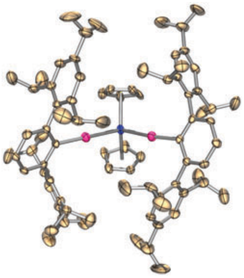
Organometallic compounds containing new Hf–Ga and Hf–In bonds: $Cp_2Hf(ER)_2$ (Cp = C_5H_5; E = Ga, In; R = $–C_6H_3$-2,6-(2,4,6-*i*-$Pr_3C_6H_2)_2$)

Brandon Quillian, Yuzhong Wang, Pingrong Wei and Gregory H. Robinson*

Sodium metal reduction of $RECl_2$ (E = Ga, In; R = $–C_6H_3$-2,6-(2,4,6-*i*-$Pr_3C_6H_2)_2$) with Cp_2HfCl_2 gives $Cp_2Hf(ER)_2$ compounds, which represent the first Hf–E bonds.



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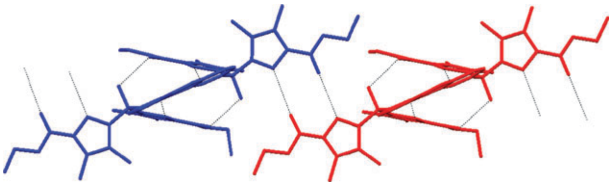
Oxidation-induced control of self-assembly using a bis-dipyrromethyl substituted phenanthroline building block

Patrick Plitt, Vincent M. Lynch and Jonathan L. Sessler*

Oxygenation of the *meso*-carbon atoms of the novel building block bis-dipyrromethyl substituted phenanthroline triggers a change in the hydrogen bond interactions from intramolecular to intermolecular.



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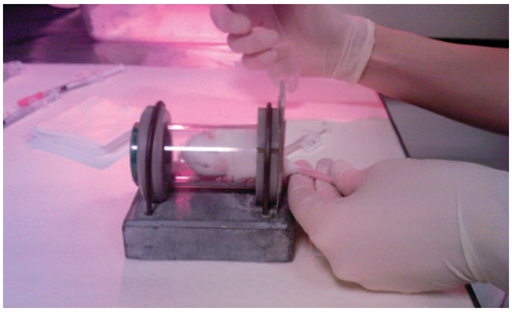
Toxicity and biodistribution of *para*-sulfonato-calix[4]arene in mice

Anthony W. Coleman,* Said Jebors, Sebastien Cecillon, Pascale Perret, Dominique Garin, Danièle Marti-Battle and Marcelle Moulin

In vivo testing of *para*-sulfonato-calix[4]arene in mice shows that the molecule has an acute toxicity at doses of 400 mg kg^{-1}; the molecule is rapidly cleared from mice in urine and does not pass the blood–brain barrier.



LETTERS

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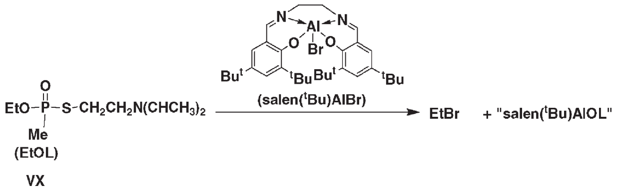
Group 13 chelates in nerve gas agent and pesticide dealkylation

Amitabha Mitra, David A. Atwood,* Jeffrey Struss, Daniel J. Williams,* Bradley J. McKinney, William R. Creasy, David J. McGarvey, H. Dupont Durst and Roderick Fry

Schiff base boron and aluminium bromides have been used to cleave organophosphate nerve agents and pesticides and their simulants.



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Intramolecular binding site competition as a means of tuning the response of a colourimetric anion sensor

Sara Jane Dickson, Emma V. B. Wallace, Adam N. Swinburne, Martin J. Paterson, Gareth O. Lloyd, Andrew Beeby, Warwick J. Belcher and Jonathan W. Steed*

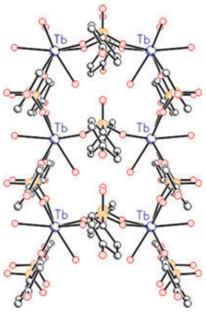
A viologen-derived double tripod receptor with pyridinium-based binding groups colourimetrically senses carboxylate ions. The number of equivalents of anion required for the onset of the colour change depends on the peripheral functional groups.

790

Synthesis and structures of luminescent ladder-like lanthanide coordination polymers of 4-hydroxybenzenesulfonate

Xiaoping Yang, Joseph H. Rivers, W. Jeffrey McCarty, Michael Wiester and Richard A. Jones*

Reaction of sodium 4-hydroxybenzenesulfonate dihydrate ($NaL \cdot 2H_2O$) with $LnCl_3 \cdot 6H_2O$ (3 : 1) in refluxing methanol gives the novel isomorphous 1-D framework compounds $\{[LnL_3(H_2O)_2] \cdot 2H_2O\}_\infty$ (Ln = Tb, Er and Yb) in 46–60% yields.



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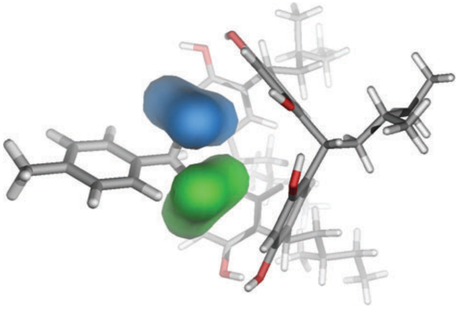
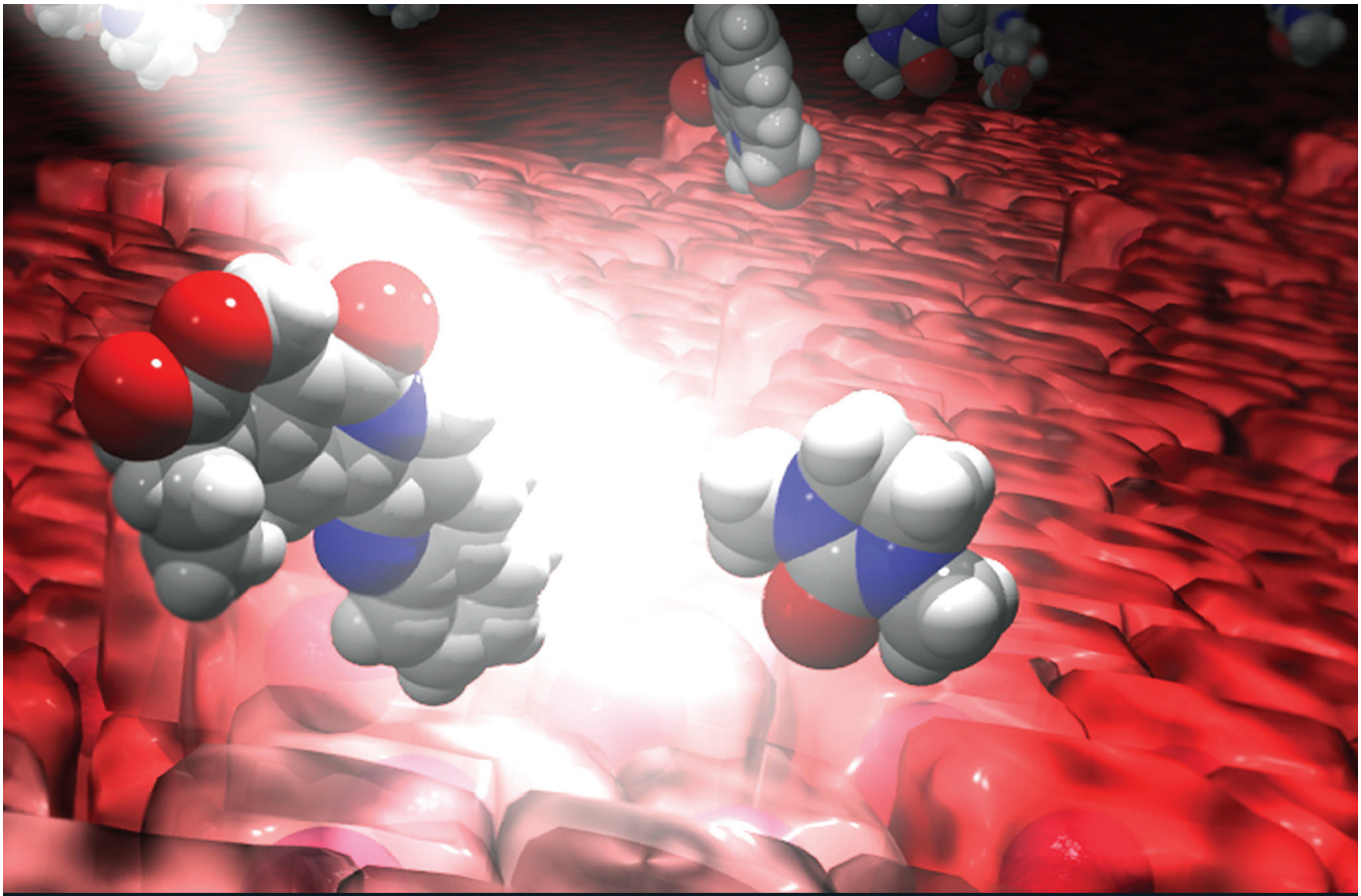
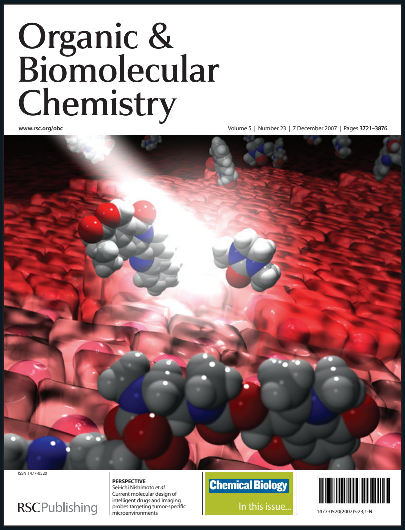
Effects of remote chiral centers on encapsulated molecules

Michael P. Schramm and Julius Rebek, Jr.*

Two homotopic methyl groups become diastereotopic when encapsulated in a chiral hybrid assembly; remotely situated chiral centers at the base of the resorcinarene relay information through space, and these effects are shown to be a function of distance.







LETTERS

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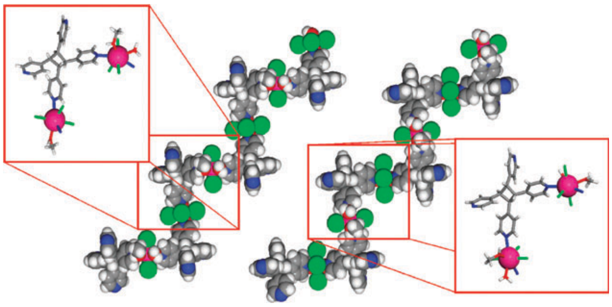
A lanthanide-based helicate coordination polymer derived from a rigid monodentate organic bridge synthesized in the solid state

Dejan-Krešimir Bučar, Giannis S. Papaefstathiou, Tamara D. Hamilton and Leonard R. MacGillivray*

A molecule synthesized in the organic solid state is shown to serve as a rigid and angular building block of a metallosupramolecular architecture, with a structure that conforms to a helicate.



PAPERS

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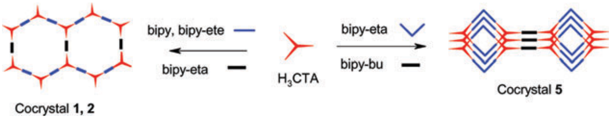
Ternary and quaternary co-crystals of 1,3-*cis*,5-*cis*-cyclohexanetricarboxylic acid and 4,4′-bipyridines

Balakrishna R. Bhogala and Ashwini Nangia*

Co-crystals of 1,3,5-cyclohexanetricarboxylic acid · 4,4′-bipyridine1 · bipyridine2 have hexagonal or square supramolecular network depending on the nature of methylene/ethene tether between the bipy groups. A self-assembly model to explain the formation of different network architectures from similar node and connector building blocks is proposed.



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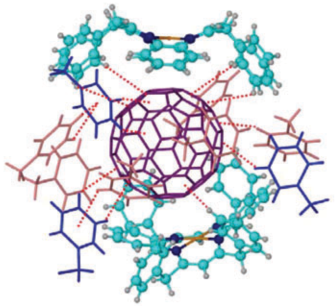
Controlling the confinement of fullerene C_{60} molecules using a saddle shape Ni(II) macrocycle

Marck Norret, Mohamed Makha, Alexandre N. Sobolev and Colin L. Raston*

Synthesis of a novel saddle-shaped Ni-macrocycle (NiTBTAA) and solid-state inclusion structure with fullerene C_{60}: interaction of sterically demanding ligand with fullerene C_{60} effect dispersion of the fullerene in a overall hexagonal array.



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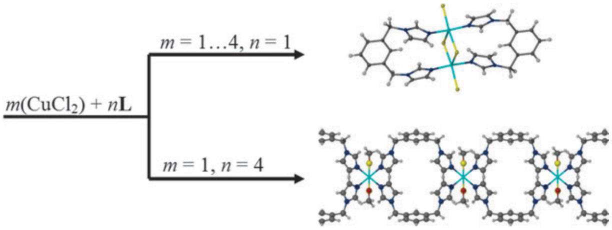
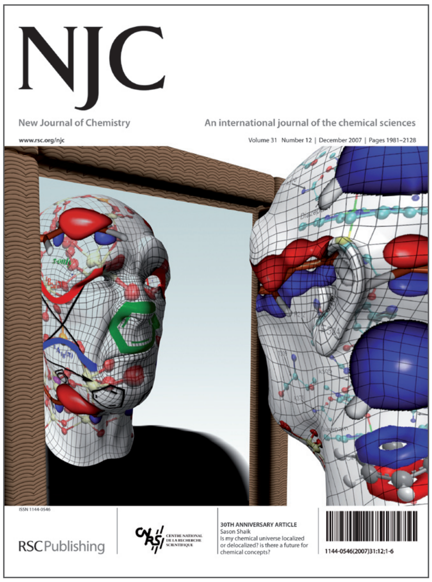
Influence of the metal-to-ligand ratio on the formation of metal organic complexes

Liliana Dobrzańska, Dewald J. Kleinhans and Leonard J. Barbour*

Three Cu(II) salts with Cl^-, Br^- or NO_3^- counterions in combination with the ditopic ligand 1,3-bis(imidazol-1-ylmethyl)benzene (**L**) were used to study the influence of the metal to ligand molar ratio on the formation of the final product. Single-crystal X-ray analysis revealed structural diversity of the products formed, ranging from discrete species to extended 1D and 2D coordination polymers.





PAPERS

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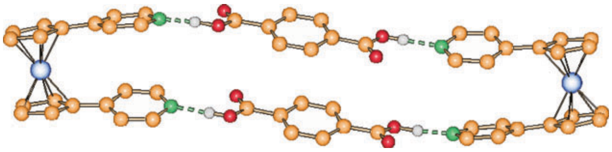
Mechanochemical assembly of hybrid organic–organometallic materials. Solid–solid reactions of 1,1′-di-pyridyl-ferrocene with organic acids

Dario Braga,* Stefano Luca Giaffreda, Fabrizia Grepioni,* Giuseppe Palladino and Marco Polito

Manual kneading of the organometallic complex [Fe(η^5-C_5H_4-$C_5H_4N)_2$] with solid fumaric, succinic, tridecanedioic, terephthalic, trimesic and thiophene-2,5-dicarboxylic acids generated the corresponding adducts, whether salts or molecular complexes.



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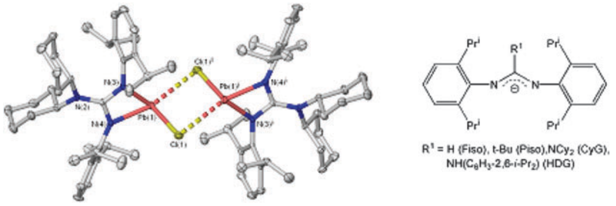
Thermally stable lead(II) amidinates and guanidinates

Andreas Stasch, Craig M. Forsyth, Cameron Jones and Peter C. Junk*

Synthetically discriminating, bulky amidinate and guanidinate ligands (A) provide stable lead(II) complexes [Pb(L)$_2$] (L = Fiso) or [Pb(L)Cl]$_2$ (L = Piso, CyG, HDG), the latter existing as loosely associated dimers in the solid state.



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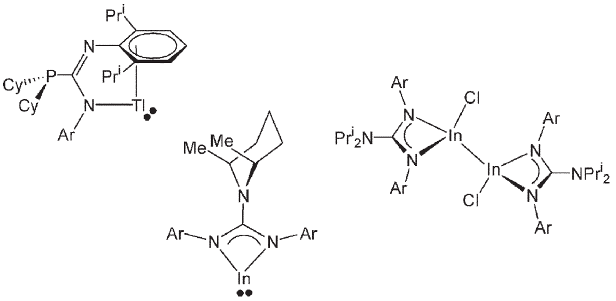
Group 13 metal(I) and (II) guanidinate complexes: effect of ligand backbone on metal oxidation state and coordination sphere

Guoxia Jin, Cameron Jones,* Peter C. Junk, Andreas Stasch and William D. Woodul

Reactions of guanidinate and phosphaguanidinate salts with group 13 metal(I) halides are reported. These have given a variety of metal(I) and (II) complexes that reveal how subtle changes to the sterics and electronics of the backbone substituents of the ligands can have a significant effect on the product obtained.



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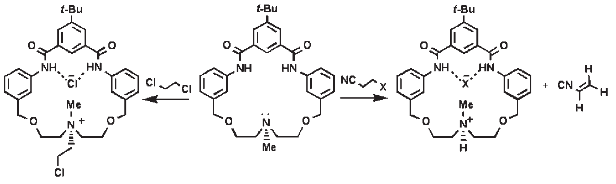
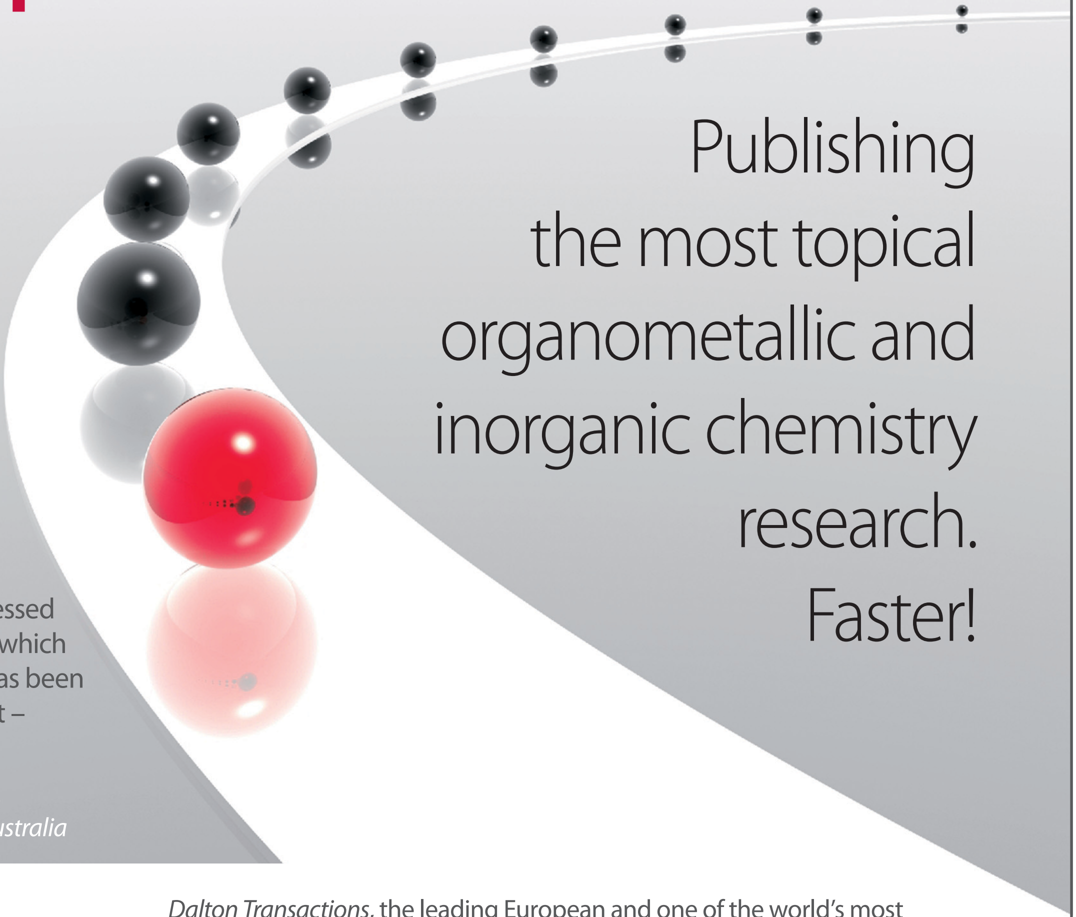
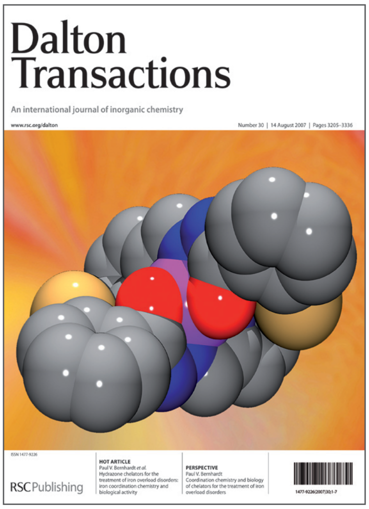
Crossing the threshold from accelerated substitution to elimination with a bifunctional macrocycle

Jeremiah J. Gassensmith, Jung-Jae Lee, Bruce C. Noll and Bradley D. Smith*

A macrocyclic amine with anion binding amide residues undergoes a highly accelerated substitution reaction with 1,2-dichloroethane but the outcome with 3-halopropionitriles is accelerated substitution.



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PAPERS

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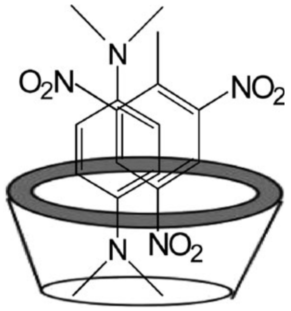
Pattern recognition based identification of nitrated explosives

Aravindan Ponnu, Nicola Y. Edwards and Eric V. Anslyn*

We report an effective approach for the identification of nitro explosives by the reaction of an electron-acceptor with an electron-donor with and without the addition of γ-cyclodextrin (γ-CD). Pattern recognition analysis was applied to analyze the data collected and it showed successful discrimination of the nitro explosives. This work represents the simplest colorimetric chemical sensor technique to be used in monitoring the range of common nitro explosives.



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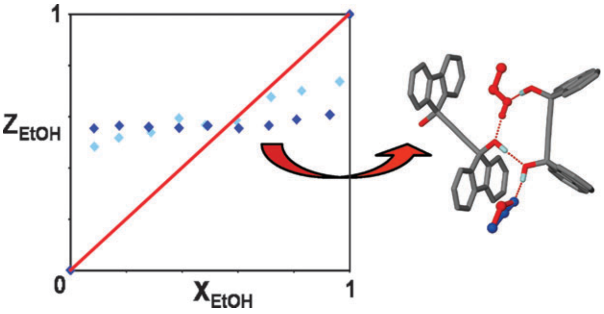
Selectivity and structure of mixed guest clathrates

Tanya le Roex,* Luigi R. Nassimbeni and Edwin Weber

Crystal structure analyses of mixed guest clathrates are correlated to their selectivity profiles giving surprising results.



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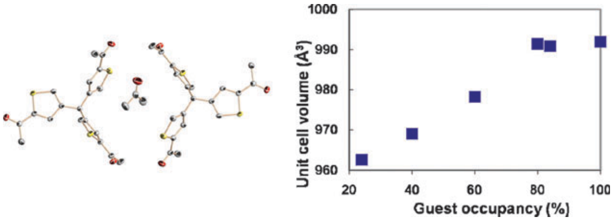
Guest capture, storage and removal in the TATM host framework: a single-crystal study

Tara J. Burchell, Gary D. Enright and John A. Ripmeester*

Herein we examine the effects of guest removal on the crystallographic parameters of TATM host–guest inclusion compounds and the degree to which simple organic guest molecules can be removed from the inclusion before framework collapse.



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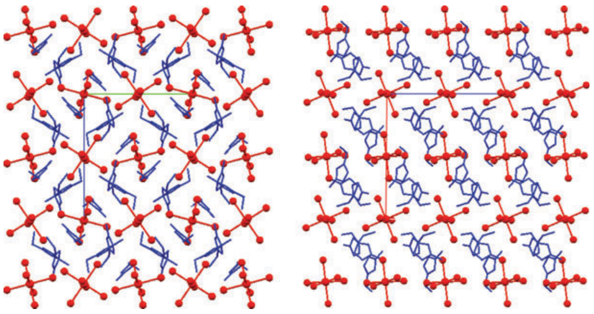
Flexible coordination environments of lanthanide complexes grown from chloride-based ionic liquids

C. Corey Hines, David B. Cordes, Scott T. Griffin, Savannah I. Watts, Violina A. Cocalia and Robin D. Rogers*

Hydrated lanthanide(III) chlorides readily dissolve in the low melting ionic liquid 1-ethyl-3-methylimidazolium chloride in an open vessel at 110 °C, and upon cooling crystallize as the anhydrous $[C_2mim]_3[LnCl_6]$.

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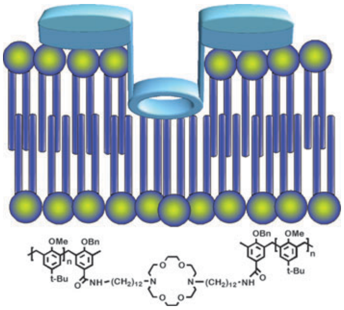

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