

# ChemComm

Chemical Communications

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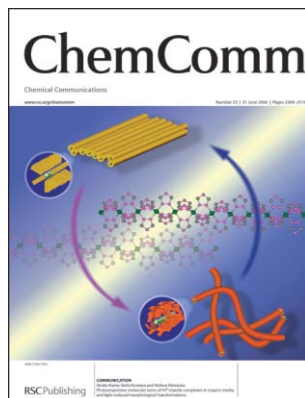
## IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (23) 2409–2516 (2006)



### Cover

See William I. F. David, Paul A. Anderson *et al.*, page 2439. Synthesis and structure of the new complex hydride  $\text{Li}_4\text{BH}_4(\text{NH}_2)_3$  solved from synchrotron X-ray and neutron powder diffraction data. Image reproduced by permission of Philip A. Chater, William I. F. David, Simon R. Johnson, Peter P. Edwards and Paul A. Anderson from *Chem. Commun.*, 2006, 2439.



### Inside cover

See Nobuo Kimizuka *et al.*, page 2442. Photoresponsive molecular wires of lipophilic  $\text{Fe}(\text{II})$  1,2,4-triazole complexes in organic media and their controlled self-assembly. Image reproduced by permission of Shoko Kume, Keita Kuroiwa and Nobuo Kimizuka from *Chem. Commun.*, 2006, 2442.

## CHEMICAL SCIENCE

C41

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, as well as the most significant scientific advances.

## Chemical Science

June 2006/Volume 3/Issue 6

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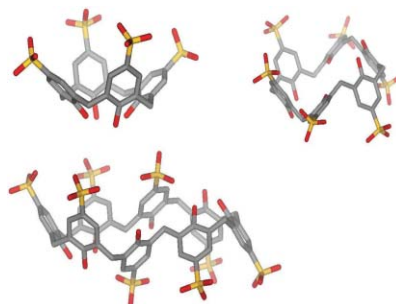
## FEATURE ARTICLE

2425

### Biochemistry of the *para*-sulfonato-calix[n]arenes

Florent Perret, Adina N. Lazar and Anthony W. Coleman\*

The biochemistry of the *para*-sulfonato-calix[n]arenes has shown rapid development during the past ten years, the highly diverse biomedical applications of these molecules now include anti-viral, anti-thrombotic activities, enzyme blocking and protein complexation. The future is even more promising as *para*-sulfonato-calix[n]arenes have, now, been shown to have potential in the diagnosis of prion-based diseases. Their innocuous nature, as far as is known at present, may open up their future use in medications.



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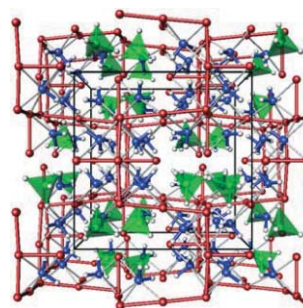
## COMMUNICATIONS

2439

### Synthesis and crystal structure of $\text{Li}_4\text{BH}_4(\text{NH}_2)_3$

Philip A. Chater, William I. F. David,\* Simon R. Johnson, Peter P. Edwards and Paul A. Anderson\*

The structure of the new complex hydride  $\text{Li}_4\text{BH}_4(\text{NH}_2)_3$  formed by the reaction of  $\text{LiBH}_4$  with  $\text{LiNH}_2$  solved by computational methods from synchrotron X-ray and neutron powder diffraction data.

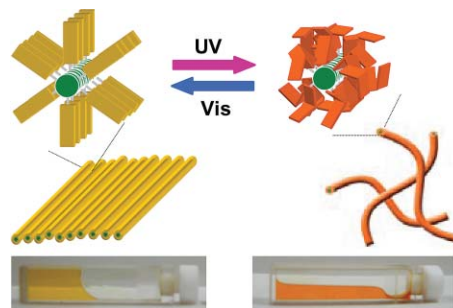


2442

### Photoresponsive molecular wires of $\text{Fe}^{\text{II}}$ triazole complexes in organic media and light-induced morphological transformations

Shoko Kume, Keita Kuroiwa and Nobuo Kimizuka\*

Photomanipulation of lipophilic 1D metal complexes leads to reversible control over morphology, assembly and the gel-to-sol transition in organic media.

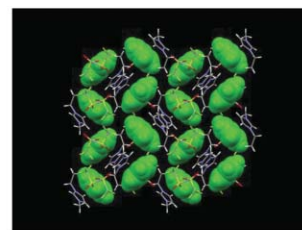
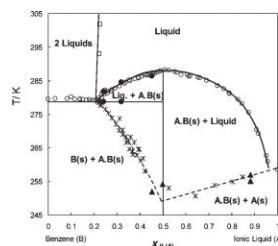


2445

### Condensed phase behaviour of ionic liquid–benzene mixtures: congruent melting of a $[\text{emim}][\text{NTf}_2] \cdot \text{C}_6\text{H}_6$ inclusion crystal

Joanna Óachwa, Isabel Bento, M. Teresa Duarte, José N. Canongia Lopes and Luís P. N. Rebelo\*

The solid–liquid phase diagram of the ionic liquid  $[\text{emim}][\text{NTf}_2]$  + benzene reveals an equimolar inclusion compound with congruent melting temperature and its X-ray structure shows the formation of tube-like structures of benzene around the ionic liquid ions.

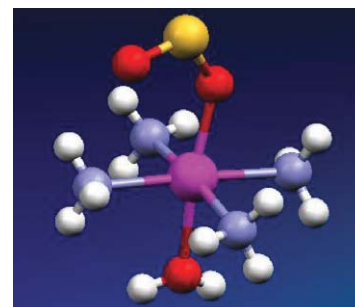


2448

### Photocrystallographic structure determination of a new geometric isomer of $[\text{Ru}(\text{NH}_3)_4(\text{H}_2\text{O})(\eta^1\text{-OSO})][\text{MeC}_6\text{H}_4\text{SO}_3]_2$

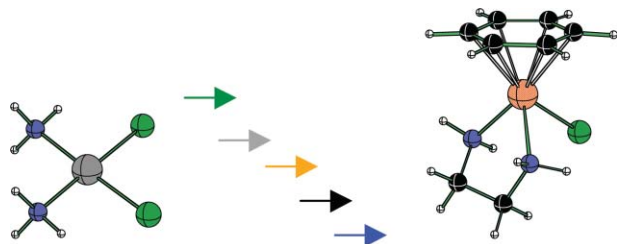
Katharine F. Bowes, Jacqueline M. Cole,\* Shamus L. G. Husheer, Paul R. Raithby,\* Teresa L. Savarese, Hazel A. Sparkes, Simon J. Teat and John E. Warren

Photocrystallographic techniques have been used to determine the crystal structure of the metastable  $\eta^1$ -OSO linkage isomer of the  $[\text{Ru}(\text{NH}_3)_4(\text{H}_2\text{O})(\text{SO}_2)]^{2+}$  cation.



## COMMUNICATIONS

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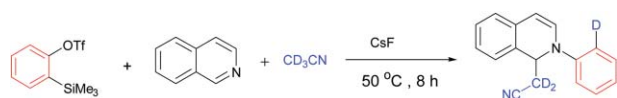


### *In silico* evolution of substrate selectivity: comparison of organometallic ruthenium complexes with the anticancer drug cisplatin

Dirk V. Deubel\* and Justin Kai-Chi Lau

A comparative quantum chemical approach helps to clarify how the selectivity of anticancer metallopharmaceuticals towards potential biological targets can be controlled by metal and ligands.

2454

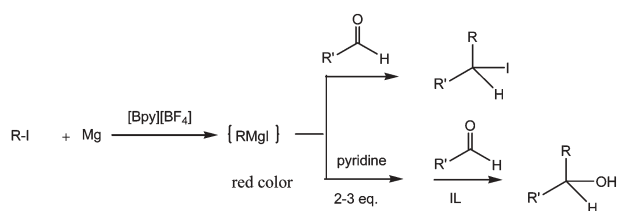


### Reaction of arynes, *N*-heteroaromatics and nitriles

Masilamani Jeganmohan and Chien-Hong Cheng\*

Various *N*-heteroaromatic compounds, including pyridines, quinolines and isoquinoline, react with arynes and nitrile-containing solvents to give *N*-arylated 1,2-dihydro-2-pyridinyl, -2-quinolinyl and -1-isoquinolinyl nitriles in excellent yields.

2457

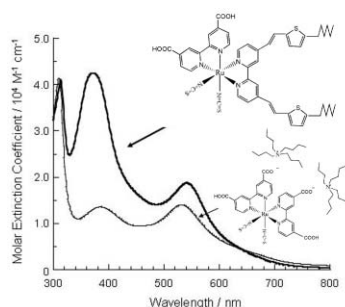


### Grignard reagents in ionic liquids

Man Chun Law, Kwok-Yin Wong and Tak Hang Chan\*

Grignard reagents were generated for the first time from magnesium and organic iodides in the ionic liquid *n*-butylpyridinium tetrafluoroborate, [bpy][BF<sub>4</sub>], and they showed different reactivity from classical Grignard reagents in organic solvents.

2460



### A novel ruthenium sensitizer with a hydrophobic 2-thiophen-2-yl-vinyl-conjugated bipyridyl ligand for effective dye sensitized TiO<sub>2</sub> solar cells

Ke-Jian Jiang, Naruhiko Masaki, Jiang-bin Xia, Shuji Noda and Shozo Yanagida\*

The novel 2-thiophen-2-yl-vinyl conjugated ruthenium sensitizer (HRS-1) shows respectable light harvesting performance in the visible-light region, giving a higher solar light-to-electricity conversion efficiency compared to the N719 sensitizer under comparable conditions.



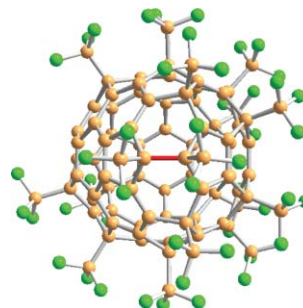
## COMMUNICATIONS

2463

### Preparation, crystallographic characterization and theoretical study of $C_{70}(CF_3)_{16}$ and $C_{70}(CF_3)_{18}$

Stanislav M. Avdoshenko, Alexey A. Goryunkov, Ilya N. Ioffe, Daria V. Ignat'eva, Lev N. Sidorov, Philip Pattison, Erhard Kemnitz and Sergey I. Troyanov\*

$C_{70}(CF_3)_{16}$  and  $C_{70}(CF_3)_{18}$  are the first  $CF_3$  fullerene derivatives to comprise a pair of adjacent  $CF_3$  groups. They have been isolated from a mixture obtained *via* reaction of  $C_{70}$  with  $CF_3I$ , characterized in a single crystal XRD study and theoretically investigated at the DFT level of theory.

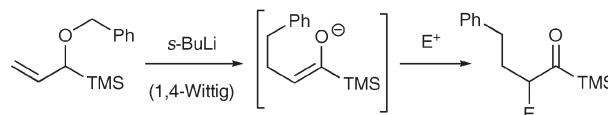


2466

### $\alpha$ -Substituted acylsilanes *via* a highly selective [1,4]-Wittig rearrangement of $\alpha$ -benzyloxyallylsilane

Edith N. Onyeozili and Robert E. Maleczka Jr.\*

After deprotonation with *s*-BuLi at cold temperatures,  $\alpha$ -benzyloxyallylsilane undergoes [1,4]-Wittig rearrangement with unprecedented selectivity to give an enolate that can be used to generate a variety of acylsilanes.

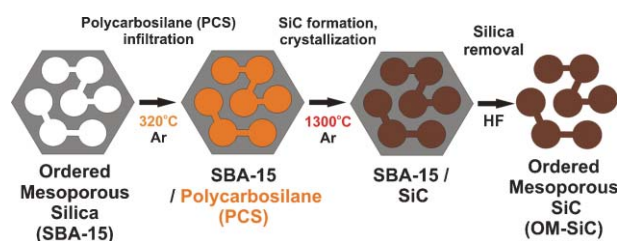


2469

### Ordered mesoporous silicon carbide (OM-SiC) *via* polymer precursor nanocasting

Piotr Krawiec, Dorin Geiger and Stefan Kaskel\*

Ordered mesoporous SiC with high specific surface area ( $650\text{--}800\text{ m}^2\text{ g}^{-1}$ ) and well ordered pore structure was obtained *via* nanocasting of polycarbosilanes into ordered mesoporous silica SBA-15 and subsequent conversion of the polymer at  $1300^\circ\text{C}$ .

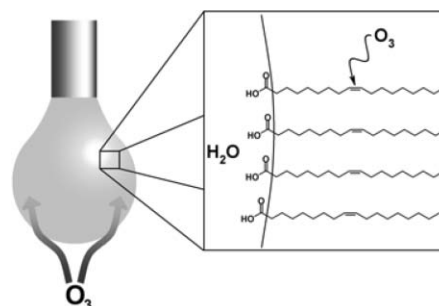


2471

### Real-time monitoring of the ozonolysis of unsaturated organic monolayers

Erick González-Labrada, Rolf Schmidt and Christine E. DeWolf\*

The reaction of ozone with unsaturated organic molecules at the air–water interface of a pendant drop was followed by axisymmetric drop shape analysis (ADSA).



## COMMUNICATIONS

2474



### The direct reaction of the *t*Bu-DAB ligand with SeCl<sub>4</sub>: a redox route to selenium–nitrogen heterocycles

Jason L. Dutton, Jocelyn J. Tindale, Michael C. Jennings and Paul J. Ragnogna\*

The reaction of SeCl<sub>4</sub> with the ubiquitous *tert*-butyl-substituted diazabutadiene ligand results in the isolation of a rare example of a 1,2,5-selenadiazolium cation, representing a novel route to Se–N ring formation. These heterocycles can be derivatised at selenium, which has led to the identification of a short Se⋯N secondary bonding interaction.

2477



### Microwave synthesis of nanocarbons from conducting polymers

Xinyu Zhang and Sanjeev K. Manohar\*

Bulk quantities of nanocarbons having pre-selected morphology can be synthesized, rapidly, and in one step, by heating doped conducting polymer precursors having similar morphology in a microwave oven, where the precursors' bulk morphology is retained upon microwave heating (spheres, fibers, tubes).

2480



### [6 + 6] Schiff-base macrocycles with 12 imines: giant analogues of cyclohexane

Joseph K.-H. Hui and Mark J. MacLachlan\*

The Schiff-base condensation reaction of 12 components in solution has yielded large hexagon-shaped conjugated macrocycles with 6 N<sub>2</sub>O<sub>2</sub> coordination sites.

2483



### *Ortho*-substituted iodobenzenes as novel organocatalysts for bromination of alkenes

D. Christopher Braddock,\* Gemma Cansell and Stephen A. Hermitage

Suitably *ortho*-substituted iodobenzenes act as catalysts for the transfer of electrophilic bromine from *N*-bromosuccinimide to alkenes as exemplified by the bromolactonisation of unsaturated aliphatic carboxylic acids.

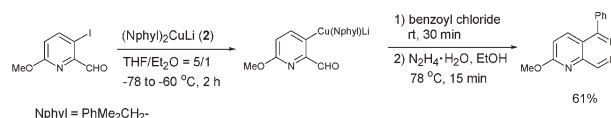
## COMMUNICATIONS

2486

### Direct preparation of copper organometallics bearing an aldehyde function *via* an iodine–copper exchange

Xiaoyin Yang and Paul Knochel\*

The iodine–copper exchange reaction allows the direct preparation of various aryl, heteroaryl and alkenyl cuprates bearing a formyl group, thus allowing a direct synthesis of polyfunctional aldehydes without the need of protecting groups or an additional oxidation step.

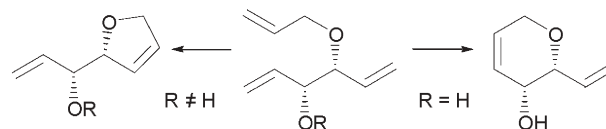


2489

### Control of ring size selectivity by substrate directable RCM

Bernd Schmidt\* and Stefan Nave

The presence or absence of a hydroxy protecting group determines the ring size selectivity of an RCM reaction. This observation suggests that hydroxy groups may exert strong catalyst-directing effects in olefin metathesis reactions.

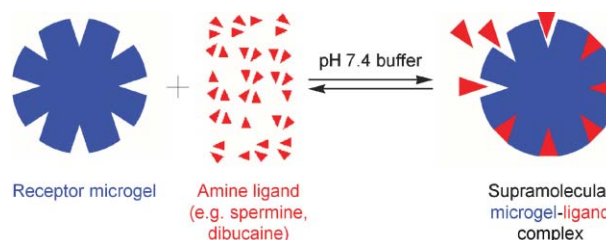


2492

### Supramolecular binding of protonated amines to a receptor microgel in aqueous medium

Alan Tominey, David Andrew, Lewis Oliphant, Georgina M. Rosair, Juliette Dupré and Arno Kraft\*

Polyanionic microgels containing negatively charged tetrazole binding sites were synthesised and showed supramolecular binding of various protonated amines (*e.g.* dibucaine, propranolol, spermine) in a competitive aqueous medium at millimolar concentration.

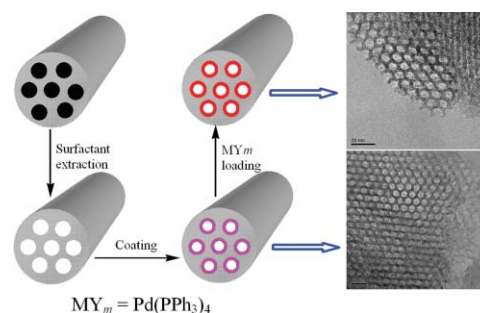


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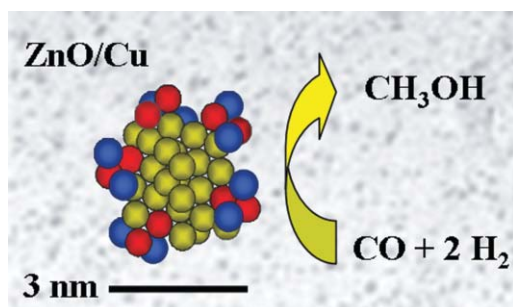
### A water-compatible, highly active and reusable PEG-coated mesoporous silica-supported palladium complex and its application in Suzuki coupling reactions

Qing Yang, Shengming Ma,\* Jixue Li, Fengshou Xiao\* and Hai Xiong

An air stable heterogeneous palladium catalyst, prepared from a coated mesoporous material containing a layer of PEG, showed very high catalytic activity for aqueous Suzuki coupling reactions.



2498

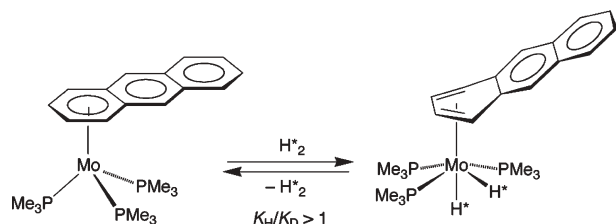


### A colloidal ZnO/Cu nanocatalyst for methanol synthesis

Marie Katrin Schröter, Lamma Khodeir, Maurits W. E. van den Berg, Todor Hikov, Mirza Cokoja, Shaojun Miao, Wolfgang Grünert, Martin Muhler and Roland A. Fischer\*

Free-standing, ZnO surface decorated Cu nanoparticles of 1–3 nm in size form stable colloids in squalane and proved to be highly active quasi homogeneous catalysts for methanol synthesis from CO and H<sub>2</sub>.

2501

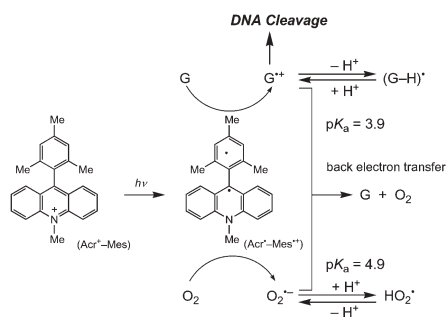


### A normal equilibrium isotope effect for oxidative addition of H<sub>2</sub> to (η<sup>6</sup>-anthracene)Mo(PMe<sub>3</sub>)<sub>3</sub>

Guang Zhu, Kevin E. Janak and Gerard Parkin\*

Oxidative addition of H<sub>2</sub> and D<sub>2</sub> to the anthracene complex (η<sup>6</sup>-AnH)Mo(PMe<sub>3</sub>)<sub>3</sub> giving (η<sup>4</sup>-AnH)Mo(PMe<sub>3</sub>)<sub>3</sub>X<sub>2</sub> (X = H, D) is characterized by a normal equilibrium isotope effect (K<sub>H</sub>/K<sub>D</sub> > 1) at temperatures close to ambient, in marked contrast to the inverse values that have been previously reported for other oxidative addition reactions.

2504

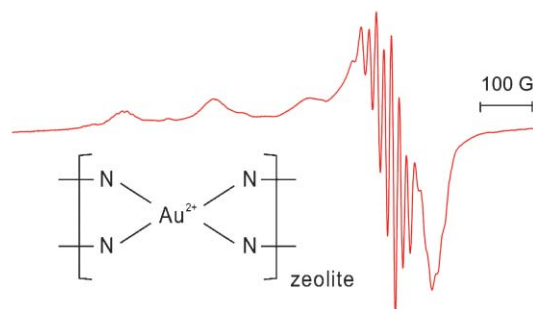


### Direct detection of nucleotide radical cations produced by electron-transfer oxidation of DNA bases with electron-transfer state of 9-mesityl-10-methylacridinium ion and resulting efficient DNA cleavage without oxygen

Kei Ohkubo, Kazusa Yukimoto and Shunichi Fukuzumi\*

Photoinduced electron transfer of DNA as well as DNA bases with 9-mesityl-10-methylacridinium ion results in formation of all types of DNA base radical cations, which have been detected as the transient absorption spectra in the laser flash photolysis measurements, leading to efficient DNA cleavage in the absence of O<sub>2</sub>.

2507



### ESR observation of the formation of an Au(II) complex in zeolite Y

Zhenping Qu, Liviu Giurgiu and Emil Roduner\*

First time observation of an Au(II) complex stabilized in a zeolite Y supercage, as evidenced by electron spin resonance (ESR). Confinement in the zeolite pores obviously prevents this unusual oxidation state from undergoing disproportionation.



## COMMUNICATIONS

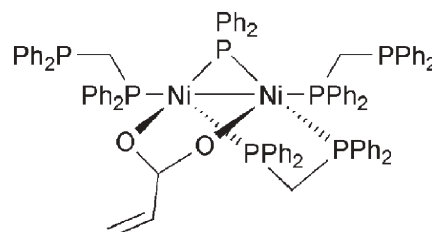
2510



### A key step in the formation of acrylic acid from CO<sub>2</sub> and ethylene: the transformation of a nickelalactone into a nickel-acrylate complex

Reinald Fischer, Jens Langer, Astrid Malassa,  
Dirk Walther,\* Helmar Görls and Gavin Vaughan

The reaction of a nickelalactone with dppm, resulting in an acrylate-bridged binuclear Ni(I) complex, models a key step in the formation of acrylic acid from CO<sub>2</sub> and ethylene.



## Chemical Biology: Directing Biosynthesis

11 - 13 September 2006, Cambridge, UK

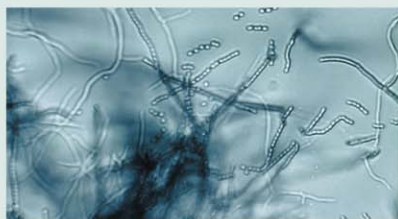
A major international conference investigating new methods for manipulating the production of novel compounds, including polyketides, non-ribosomal peptides and other natural products.

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Hans-Knöll-Institute, Germany  
Peter Leadlay  
University of Cambridge, UK

Rolf Müller  
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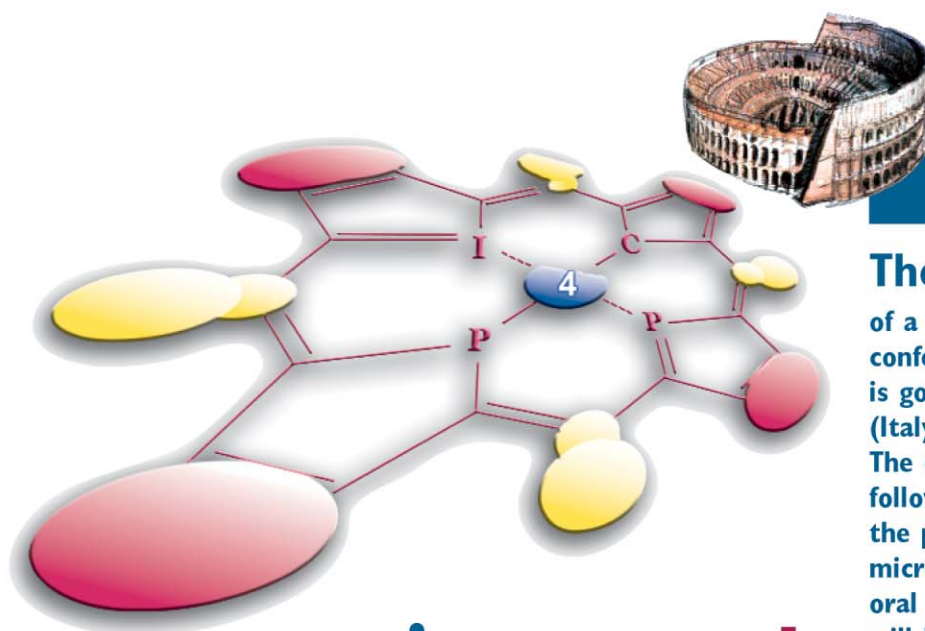
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Rome, July 2-7, 2006

icpp-4

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University of Rome "Tor Vergata"  
Society of Porphyrins and Phthalocyanines

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The conference will highlight innovative ideas and latest developments encompassing all areas of tetrapyrrole chemistry, physics, biology and medicine, with a special attention devoted to new developments and emerging technologies. The conference web page <http://icpp.uniroma2.it>, will provide the most current information about the meeting and venue.

Selected venue, the Angelicum Pontifical University of St. Thomas, Rome, is hosted in a Dominican monastery built in the XVI century on the Quirinale hill. It is at few hundred meters from Piazza Venezia adjacent to the Foro Romano: the largest archaeological area in the world.

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