IN THIS ISSUE

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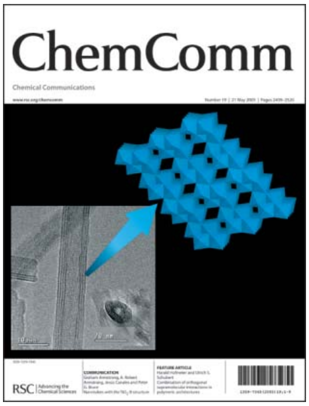
In this issue...

The feature article in this issue reviews the use of molecular recognition strategies to control supramolecular polymer structure and properties. See Harald Hofmeier and Ulrich S. Schubert, pp 2423–2432.



Cover
See Peter G. Bruce *et al.*, page 2454.
The cover image depicts titanium dioxide (TiO_2-B) nanotubes magnified 1 million times.
Image reproduced by permission of Graham Armstrong, A. Robert Armstrong, Jesús Canales and Peter G. Bruce, *Chem. Commun.*, 2005, 2454.

CHEMICAL TECHNOLOGY

FEATURE ARTICLE

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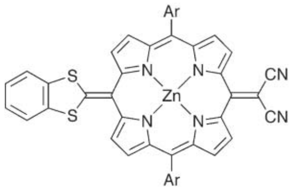
COMMUNICATIONS

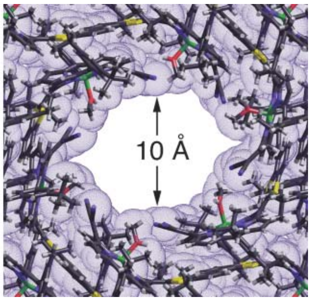
2433

Synthesis and crystal structure of a push–pull quinoidal porphyrin: a nanoporous framework assembled from cyclic trimer aggregates

Martin J. Smith, William Clegg, Kiet A. Nguyen, Joy E. Rogers, Ruth Pachter, Paul A. Fleitz and Harry L. Anderson*

A quinoidal porphyrin has been synthesised with such a curved π-system that π–π stacking leads to the formation of cyclic trimer aggregates in the crystal, which pack to generate cylindrical channels with an internal diameter of 1.0 nm.



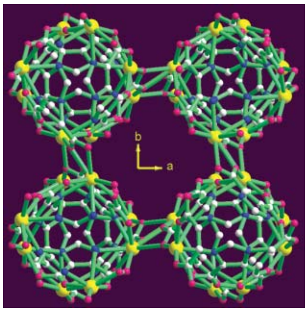


2436

Porous lanthanide–organic framework with zeolite-like topology

Tapas Kumar Maji, Golam Mostafa, Ho-Chol Chang and Susumu Kitagawa*

Novel 3D zeolite-like open frameworks, $\{[Ln_2(imidc)_2(H_2O)_3](H_2O)\}_n$, [Ln = Gd(III), Er(III)] (imidc = 4,5-imidazoledicarboxylic acid) have been hydrothermally synthesized and structurally characterized, showing structural transformation upon dehydration and highest affinity towards water molecules among a number of adsorbates.

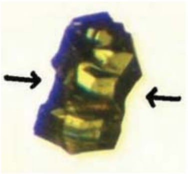


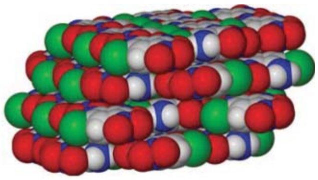
2439

Sorting of polymorphs based on mechanical properties. Trimorphs of 6-chloro-2,4-dinitroaniline

C. Malla Reddy, Srinivas Basavoju and Gautam R. Desiraju*

Shearing of crystals of a layered polymorph is used to separate it from two other crystal forms.



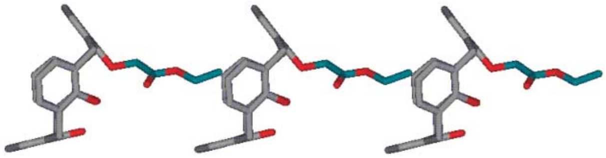


2442

Head-to-tail self-assembly of a calix[4]arene inclusion polymer controlled by a pendant arm

Sebastien Cecillon, Adina Lazar, Oksana Danylyuk, Kinga Suwinska, Beth Rather, Michael J. Zaworotko and Anthony W. Coleman*

A calix[4]arene functionalized at one phenolic group with a pendant ethoxy acetate group, forms an inclusion complex that is stable even in the presence of other potential guest molecules.



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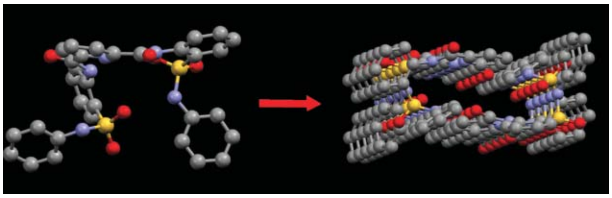
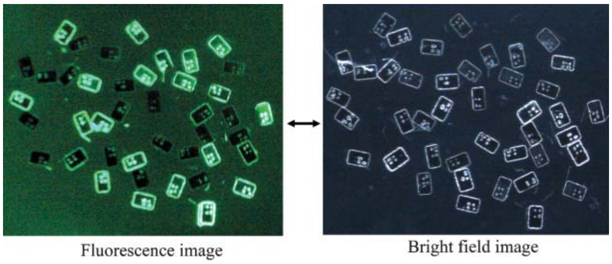


A novel self-assembled organic tubular structure

Zhi-Qiang Hu and Chuan-Feng Chen*

A novel organic tube with the walls consisting of aromatic rings was constructed by the self-assembly of a two-dimensional sheet-like molecule in the solid state.

2448



Fluorescence image

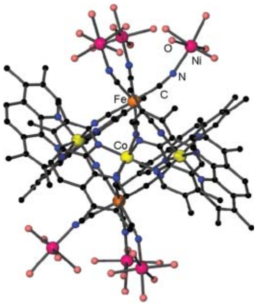
Bright field image

Microfabrication of encoded microparticle array for multiplexed DNA hybridization detection

Zheng-liang Zhi,* Yasutaka Morita, Shouhei Yamamura and Eiichi Tamiya

A strategy for the high-sensitivity, high-selectivity, and multiplexed detection of oligonucleotide hybridizations has been developed with an encoded Ni microparticle random array that was manufactured by a "top-down" approach using micromachining and microfabrication techniques.

2451

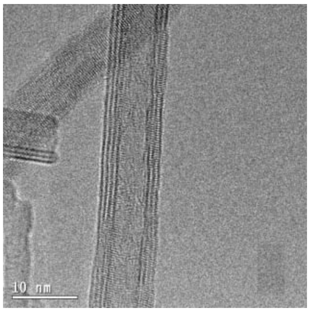


The step-wise assembly of an undecanuclear heterotrimetallic cyanide cluster

Curtis P. Berlinguette and Kim R. Dunbar*

The step-wise assembly of the high nuclearity cluster, $\{[Ni^{II}(H_2O)_5]_6[Co^{III}(tmphen)_2]_3[Fe^{II}(CN)_6]_2\}^{13+}$, is achieved by treating $\{[Co(tmphen)_2]_3[Fe(CN)_6]_2\}$ with six equivalents of $Ni(ClO_4)_2$ in aqueous MeOH.

2454



Nanotubes with the TiO_2-B structure

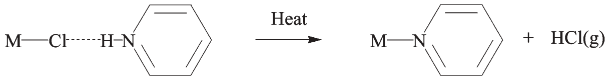
Graham Armstrong, A. Robert Armstrong, Jesús Canales and Peter G. Bruce*

First synthesis of TiO_2-B nanotubes, and by a simple hydrothermal route is reported; lithium may be intercalated up to a composition of $Li_{0.98}TiO_2$ compared with $Li_{0.91}TiO_2$ for the corresponding nanowires.

2457

Thermal solid state synthesis of coordination complexes from hydrogen bonded precursors

Christopher J. Adams, Paul C. Crawford, A. Guy Orpen,* Thomas J. Podesta and Benjamin Salt

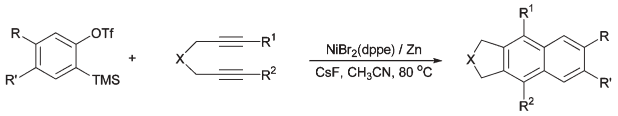


Thermal dehydrochlorination of crystalline 4-picolinium salts of $[PtCl_4]^{2-}$ and $[PdCl_4]^{2-}$ under N_2 at 160 °C leads to formation of *trans*-$[MCl_2(4\text{-picoline})_2]$ (M = Pt, Pd). In the platinum case an intermediate crystalline phase, $[4\text{-picolinium}][PtCl_3(4\text{-picoline})]$, can be isolated.

2459

Nickel-catalyzed cocyclotrimerization of arynes with diynes; a novel method for synthesis of naphthalene derivatives

Jen-Chieh Hsieh and Chien-Hong Cheng*



The $NiBr_2(dppe)$–Zn system effectively catalyzes the [2 + 2 + 2] cocyclotrimerization of arynes with diynes, leading to substituted naphthalene derivatives in moderate to good yields. This cocyclotrimerization reaction shows excellent tolerance of functional-group and fused-ring size.

2462

Benzene C–H activation by platinum(II) complexes of bis(2-diphenylphosphinophenyl)amide

Lan-Chang Liang,* Jia-Ming Lin and Wei-Ying Lee

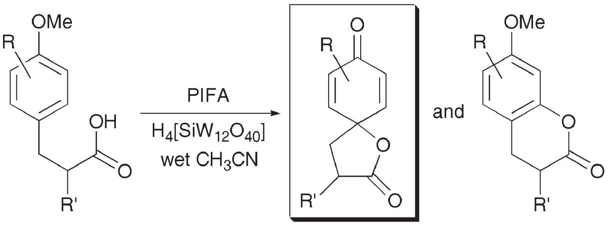
$$[PNP]PtMe \xrightarrow[\text{RT}]{B(C_6F_5)_3,\ C_6H_6} [PNP]PtPh \xleftarrow[\text{heat}]{NEt_3,\ C_6H_6} [PNP]PtOTf$$

The amido diphosphine complexes [PNP]PtMe and [PNP]PtOTf, where $[PNP]^-$ is bis(2-diphenylphosphinophenyl)amide, effectively activate the benzene C–H bond in the presence of an appropriate Lewis acid or base, leading to the formation of [PNP]PtPh quantitatively.

2465

A new synthesis of dienone lactones using a combination of hypervalent iodine(III) reagent and heteropoly acid

Kayoko Hata, Hiromi Hamamoto, Yukiko Shiozaki and Yasuyuki Kita*

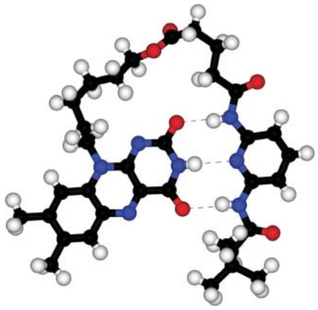


R = alkyl, alkoxy

high yield and high selectivity

A combination of hypervalent iodine(III) reagent, phenyliodine(III) bis(trifluoroacetate) (PIFA), and heteropoly acid (HPA) provide a new oxidative route to dienone lactones from non-phenolic alkanoic acid derivatives.

2468

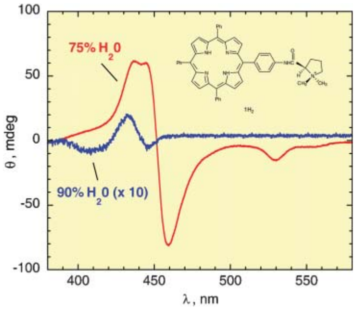


Model systems for flavoenzyme activity: a tuneable intramolecularly hydrogen bonded flavin–diamidopyridine complex

Alan S. F. Boyd, Joseph B. Carroll, Graeme Cooke,* James F. Garety, Brian J. Jordan, Suhil Mabruk, Georgina Rosair and Vincent M. Rotello

We report the electrochemically and thermally tuneable intramolecular hydrogen bonding interactions between a covalently linked flavin–diamidopyridine unit.

2471

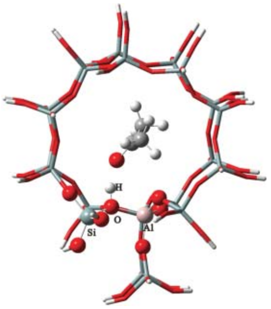


Supramolecular chirality control by solvent changes. Solvodichroic effect on chiral porphyrin aggregation

Donato Monti,* Mariano Venanzi, Giovanna Mancini, Corrado Di Natale and Roberto Paolesse

The solvent composition strongly influences the morphology of chirally functionalised porphyrin aggregates. This results in the tuning of the supramolecular chirality of the obtained architectures.

2474

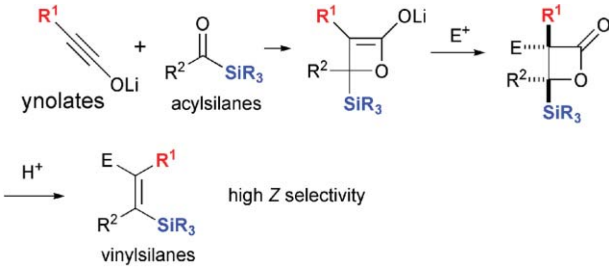


Prediction of the ^{13}C NMR chemical shifts of organic species adsorbed on H-ZSM-5 zeolite by the ONIOM-GIAO method

Anmin Zheng, Lei Chen, Jun Yang, Yong Yue, Chaohui Ye, Xin Lu and Feng Deng*

The ONIOM-GIAO method has been used to accurately predict ^{13}C NMR chemical shifts for a series of organic species adsorbed on H-ZSM-5 zeolite. This is useful for the spectroscopic identification of complicated catalytic systems.

2477



A synthesis of multisubstituted vinylsilanes *via* ynolates: stereoselective formation of β-silyl-β-lactones followed by decarboxylation

Mitsuru Shindo,* Kenji Matsumoto and Kozo Shishido

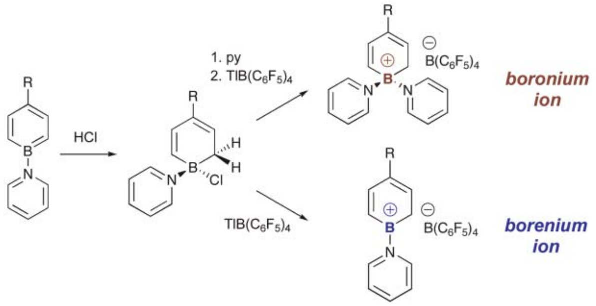
(*Z*)-Selective synthesis of multisubstituted vinylsilanes was achieved by stereoselective protonation or alkylation of β-silyl-β-lactone enolates, prepared by cycloadditions of acylsilanes with ynolates, followed by decarboxylation.

2480

Cyclic boronium and borenium cations derived from borabenzene–pyridine complexes

Ioan Ghesner, Warren E. Piers,* Masood Parvez and Robert McDonald

A new class of elusive boronium and borenium ions are derived from borabenzene pyridine adducts *via* protonation and ionization. Their potential role in the chemistry of borabenzene chemistry is discussed.

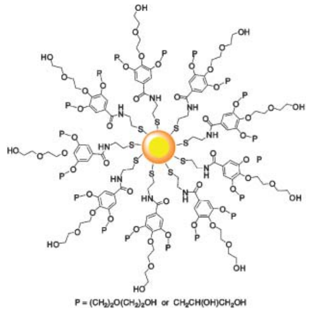


2483

Diethylene glycol ether-linked 3,4,5-trihydroxybenzamides as triply branched dendritic anchors to CdSe/ZnS core/shell type nanoparticles: potential hydrophilic fluorescent probes

Chien-Tien Chen,* Vijay D. Pawar, Yogesh S. Munot, Chia-Chun Chen* and Chih-Jung Hsu

Hydrophilic nanohybrids where dendritic gallamides bearing a thiol anchoring group with attached ethylene glycol unit(s) toward the periphery are employed to overcoat CdSe/ZnS core/shell nanoparticles.

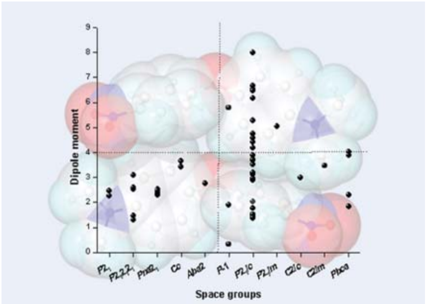


2486

Correlation between molecular dipole moment and centrosymmetry in some crystalline diphenyl ethers

Archan Dey and Gautam R. Desiraju*

The presence of a large molecular dipole moment in diphenyl ethers leads unequivocally to a centrosymmetric crystal structure.

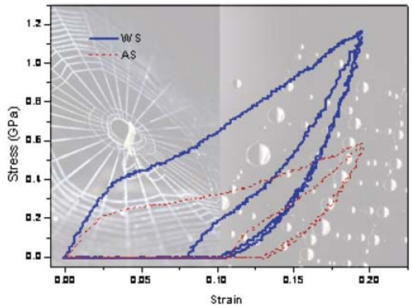


2489

Extended wet-spinning can modify spider silk properties

Yi Liu, Zhengzhong Shao* and Fritz Vollrath

Because of its outstanding mechanical properties, the study of spider silks has recently become a major subject for the study of biopolymer structure and function including the experimental interference with the natural spinning procedure. Here we study the effect of spinning through a water bath and demonstrate that this makes for a stiffer silk, despite the old observation that bathing a finished silk fibre typically has the opposite effect.



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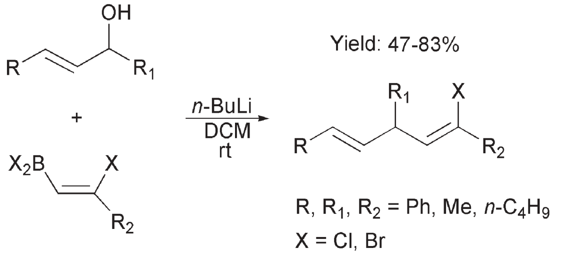
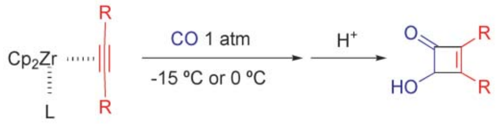


Alkenylation of allylic alcohols using alkenylboron dihalides: a formal transition-metal free Suzuki reaction

George W. Kabalka,* Min-Liang Yao, Scott Borella and Zhongzhi Wu

Carbon–carbon bond formation *via* substitution of an allylic hydroxide with stereodefined alkenyl groups using alkenylboron dihalides in the absence of transition metals.

2495

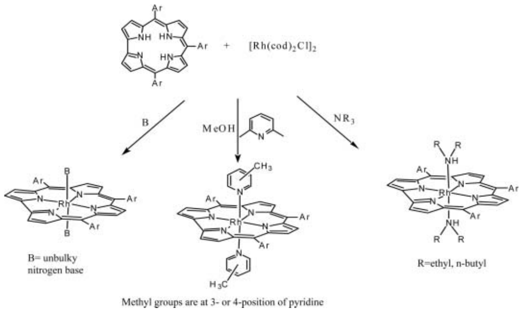


Double carbonylation of zirconocene–alkyne complexes

Shizue Mito and Tamotsu Takahashi*

Zirconocene–alkyne complexes prepared from Cp_2ZrBu_2, phosphines and alkynes reacted with CO to give double carbonylation products, 4-hydroxycyclobuten-1-one derivatives after hydrolysis.

2497

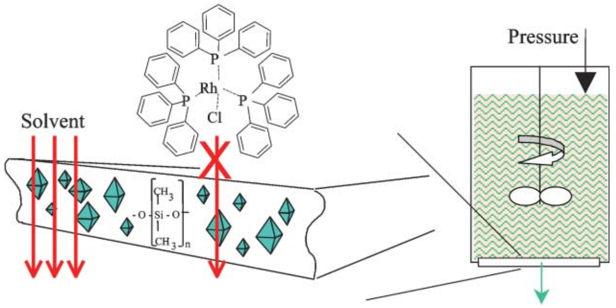


Synthesis and characterization of Rh^{III} corroles: unusual reactivity patterns observed during metalation reactions

James P. Collman,* Hong J. H. Wang,
Richard A. Decreau, Todd A. Eberspacher and
Christopher J. Sunderland

A facile approach to the synthesis of a series of Rh^{III} corrole complexes is developed. Unusual activation of C–C and C–N bonds in bulky bases is observed during metalation reaction. It is found that the activation is associated with the steric bulkiness of the base that is used.

2500



Zeolite filled polydimethylsiloxane (PDMS) as an improved membrane for solvent-resistant nanofiltration (SRNF)

Lieven E. M. Gevers,* Ivo F. J. Vankelecom and Pierre A. Jacobs

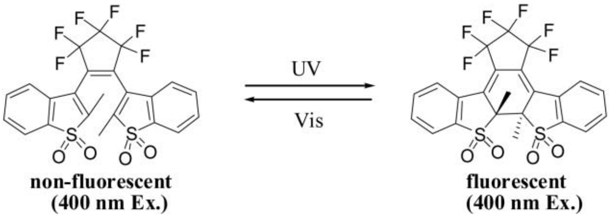
The use of zeolite-filled polydimethylsiloxane membranes in solvent-resistant nanofiltration significantly extends the possibilities for this technique in novel applications involving strongly swelling organic solvents and increased temperatures.

2503

Highly fluorescent photochromic diarylethene in the closed-ring form

Yong-Chul Jeong, Sung Ik Yang,* Kwang-Hyun Ahn* and Eunkyoung Kim*

A highly fluorescent diarylethene in the closed-ring form was synthesized by the oxidation of 1,2-bis(2-methyl-1-benzothiophene-3-yl)perfluorocyclopentene (BTF6).

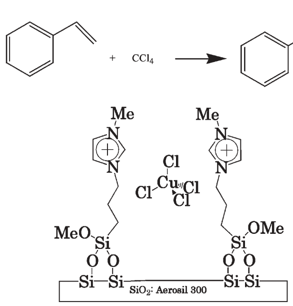


2506

Immobilized metal ion-containing ionic liquids: preparation, structure and catalytic performance in Kharasch addition reaction

Takehiko Sasaki, Chongmin Zhong, Mizuki Tada and Yasuhiro Iwasawa*

The immobilized Cu^{2+}-containing ionic liquid catalyst with a sandwiched [$CuCl_4^{2-}$] moiety promotes the Kharasch addition reaction between styrene and CCl_4 with good and reusable performance.

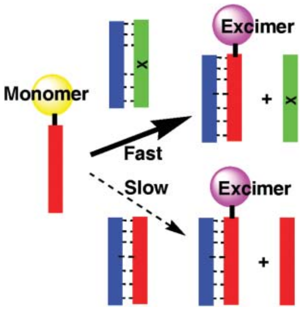


2509

DNA mismatch detection using a pyrene–excimer-forming probe

Kazushige Yamana,* Yudai Fukunaga, Yusuke Ohtani, Sayaka Sato, Mitsunobu Nakamura, Won Jong Kim, Toshihiro Akaike and Atsushi Maruyama

A pyrene–excimer-forming probe allowed the easy and sensitive detection of a single base mismatch in target DNA. This was due to the faster strand exchange rate compared to a fully-matched target.

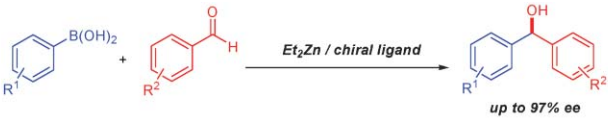


2512

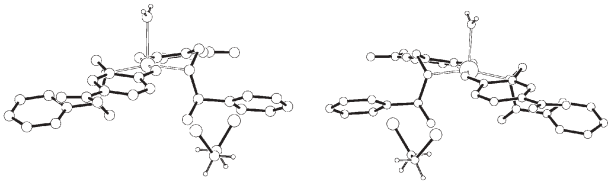
Catalytic enantioselective arylation of aldehydes: boronic acids as a suitable source of transferable aryl groups

Antonio L. Braga,* Diogo S. Lüdtke, Fabrício Vargas and Marcio W. Paixão

The catalytic enantioselective arylation of aldehydes using boronic acids as the source of transferable aryl groups is described. The reaction proceeds in excellent yields and high enantioselectivities (up to 97% ee) in the presence of a chiral amino alcohol.



2515



Enantiospecific inclusion of chiral 1,2-dichloroethane rotamers in the crystal lattice of chiral square-pyramidal Cu(II) complexes with perfectly polar alignment of guest and host molecules

Vamsee Krishna Muppidi, Panthapally S. Zacharias* and Samudranil Pal*

Two Cu(II) complexes ([$CuL_2(H_2O)$], L^- = *R*- and *S*-forms of a bidentate chiral ligand) form 1 : 1 host–guest crystals with $ClCH_2CH_2Cl$. Intermolecular H-bonding leads to enantioselective trapping of guest rotamers and polar order of host and guest molecules.

AUTHOR INDEX

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CALL FOR PROPOSALS
FOR
COST CHEMISTRY ACTION D33

"Nanoscale Electrochemical and Bio-processes (Corrosion) at Solid-aqueous Interfaces of Industrial Materials"

The new COST Action D33 was launched with the general objective: *To develop the understanding of biochemical processes at solid-aqueous interfaces leading to a universal approach for understanding biofouling related issues.*

Priority scientific topics, which could be the subjects of Working Groups, are:

(1) Development, adaptation and coupling of surface science methods for an improved analysis of the chemical processes occurring at the interfaces between materials and (micro) organisms,
(2) Analyses of chemical and biological processes causing adhesion of macromolecules, (microbial) cells, consortia etc to materials surfaces,
(3) Understanding of the elementary steps leading to biocorrosion, biofouling, biofilms (also in health related environments or food industry), bioleaching etc in order to inhibit or improve the respective processes.

Other relevant scientific topics which relate to the subjects defined in the Memorandum of Understanding (MoU) will be considered.

The Management Committee of the COST Action D33 seeks submissions of Working Group proposals for high-quality research collaborations.

Working Groups (WG) should be designed to carry out a collaborative research in areas relevant to the objectives and scientific priorities of D33. In practice, the collaboration between WG members will lead to new scientific results by means of combining their complementary expertise and experimental or theoretical techniques and approaches, within shared scientific interests and goals. WG proposals must be submitted by partners from at least three different COST-member states but preferably at least five different members states (here a member state is defined as one of the 35 COST member states), which have signed (or will have signed at time of the start of the proposal) the MoU. WGs should include one partner from any member state; in larger WGs two partners from the same member state can be accepted. WGs with more than ten partners are usually not efficient and will not be encouraged. All persons from universities, public sector or industries, who undertake research, are eligible to apply for participation in a COST Action. Proposals should be oriented towards fundamental or pre-competitive research. They will be peer-reviewed and subjected to the decision of the Management Committee. Proposals can be submitted anytime in the course of the first half of the D33 term that is until mid 2007.
The first proposals will be considered at the MC meeting at the beginning of December 2005. To this end, early submissions till the end of September 2005 are strongly encouraged. They should be sent to the D33 Chair (wolfgang.sand@uni-due.de) and the COST Office Science Officer (dneibecker@cost.esf.org).
The procedure for submitting a WG proposal can be downloaded from the COST Chemistry web site at http://costchemistry.epfl.ch (under "Working Group Proposals" and under "Download forms" click on "COST Chemistry Working Group Proposal Form") or from the COST web site at http://cost.cordis.lu. The Technical Annex of the D33 MoU, which states in detail the D33 objectives and scientific priorities, is also available from these COST web sites.

Rating Criteria of WG Proposals

- Relevance to the objectives
- Research performance
- Innovative character (scientific quality and novelty)
- Benefits from cooperation and synergism
- Feasibility and competence of the participants