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ISSN 1144-0546 CODEN NJCHES 34(2) 173-368 (2010)



Cover

See Domenico M. Grasso et al., pp. 200-207. Are fibrils involved in Langerhans' β -cell death? Image reproduced by permission of Domenico M. Grasso from New Journal of Chemistry, 2010, 34, 200.



Inside cover

See Qian-Shu Li and R. Bruce King et al., pp. 208-214. The tetranuclear iron carbonyls $Fe_4(CO)_n$ (n = 16, 15, 14) are predicted to have low energy structures with rhombus, planar butterfly, and tetrahedral arrangements of the central Fe₄ cluster. Image reproduced by permission of R. Bruce King from New Journal of Chemistry, 2010, 34, 208.

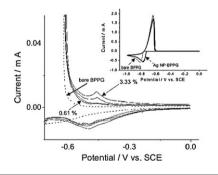
LETTERS

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Thallium underpotential deposition on silver nanoparticles: size-dependent adsorption behaviour

Fallyn W. Campbell, Yi-Ge Zhou and Richard G. Compton*

In this letter we report the size-dependent underpotential deposition (UPD) of thallium on silver nanoparticles (AgNPs); UPD of thallium is observed at bulk silver electrode and AgNPs of diameter greater than 50 nm but absent at smaller AgNPs.



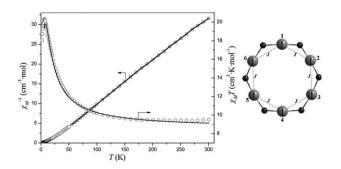


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A novel large Ni-azido circle with tridentate (NNO) Schiff base co-ligands: hexagonal structure and ferromagnetic properties

Baiwang Sun,* Xiaodan Chen, Zhongshu Li, Lei Zhang and Qihua Zhao

The title complex has a nearly hexagonal geometry with large Ni-N-Ni angles of about 127(1)°. A study of its magnetic properties showed that although it is ferromagnetic, its exchange coupling constant is very small.



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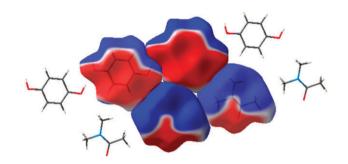
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Three new co-crystals of hydroguinone: crystal structures and Hirshfeld surface analysis of intermolecular interactions

Henrik F. Clausen, Marie S. Chevallier, Mark A. Spackman and Bo B. Iversen*

Hirshfeld surface analysis is used to study the intermolecular interactions in three new co-crystals of hydroquinone. The analysis demonstrates the importance of electrostatic complementarity for packing of molecules in crystals.

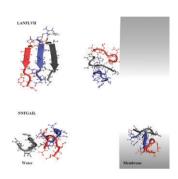


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Are fibril growth and membrane damage linked processes? An experimental and computational study of IAPP₁₂₋₁₈ and IAPP₂₁₋₂₇ peptides

Michele F. M. Sciacca, Matteo Pappalardo, Francesco Attanasio, Danilo Milardi, Carmelo La Rosa and Domenico M. Grasso*

This work demonstrates that if neutral peptides and lipids are employed, the most fibrillogenic peptide (LANFLVH) has the lowest membrane damaging effect whilst the most membrane active peptide (NNFGAIL) is less prone to form ordered amyloid-like structures.

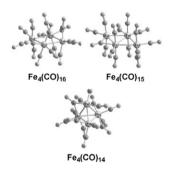


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Neutral homoleptic tetranuclear iron carbonyls: why haven't they been synthesized as stable molecules?

Ting Ting Shi, Qian-Shu Li,* Yaoming Xie, R. Bruce King* and Henry F. Schaefer III

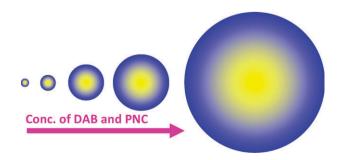
Tetranuclear iron carbonyls $Fe_4(CO)_n$ (n = 16, 15, 14) are predicted to have low energy structures with rhombus, planar butterfly, and tetrahedral arrangements of the central Fe₄ cluster and Fe-Fe single bond distances. An alternative low energy planar butterfly Fe₄(CO)₁₄ structure is also found with one short double bond Fe=Fe distance.

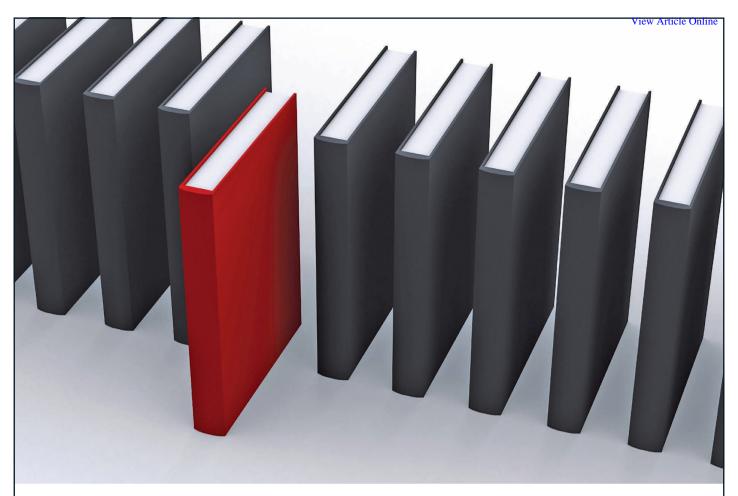


Simple systematic synthesis of size-tunable covalent organophosphonitridic framework nano- and microspheres

Paritosh Mohanty and Kai Landskron*

Monodispersed covalent organophosphonitridic framework nano- and microspheres of sizes from 80 nm to 1.5 μm were synthesized by varying the concentration of the reactants hexachlorocyclotriphosphazene (PNC) and 3,3'-diaminobenzidine (DAB) in DMF at a temperature of 125 °C in the presence of polyvinyl pyrrolidone.





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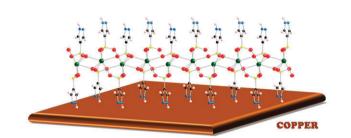


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Cation effect on the inorganic-organic layered structure of pyrazole-4-sulfonate networks and inhibitory effects on copper corrosion

Isurika R. Fernando, Nikos Daskalakis, Konstantinos D. Demadis* and Gellert Mezei*

Pyrazole-4-sulfonic acid is a versatile ligand that participates in various supramolecular interactions leading to a wide structural variety of its layered inorganic-organic metal complexes, as well as to reduced copper corrosion.



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Cyclisation reactions of some pyridazinylimidoylketenes

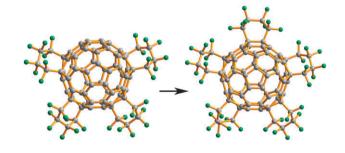
Alexander P. Gaywood, Lawrence Hill, S. Haider Imam, Hamish McNab,* Gabor Neumajer, William J. O'Neill and Péter Mátyus*

Flash vacuum pyrolysis (FVP) of the aminopyridazinone derivatives of Meldrum's acid at 600 °C (0.02 Torr) results in generation of an imidoylketene intermediate followed by cyclisation. The 4-amino compounds shown lead to mixtures of pyrido[2,3-d]pyridazines and pyrrolo[3,2-c]pyridazines. A suggested mechanism for the formation of the latter is supported by DFT calculations.

Synthesis and structure of cycloperfluoroalkylated derivatives of C_{70} , $C_{70}(C_2F_4)$ and $C_{70}(C_4F_8)_n$, n = 1-6

Natalia I. Gruzinskaya, Andrey I. Silin, Anna S. Pimenova, Pavel A. Khavrel, Vitaliy Yu. Markov, Lev N. Sidorov, Erhard Kemnitz and Sergey I. Troyanov*

Molecular structures of new cycloperfluoroalkylated C₇₀, $C_{70}(C_2F_4)$, $C_{70}(C_4F_8)$, $C_{70}(C_4F_8)_2$, $C_{70}(C_4F_8)_4$, $C_{70}(C_4F_8)_5$, and C₇₀(C₄F₈)₆ were determined by single crystal X-ray diffraction and discussed in terms of their addition patterns, relative energies, and possible formation pathways (see picture).

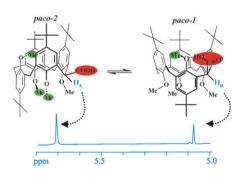


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Conformational behaviour and first crystal structures of a calix[4] arene featuring a laterally positioned carboxylic acid function in unsolvated and solvent-complexed forms

Tobias Gruber, Margit Gruner, Conrad Fischer, Wilhelm Seichter, Petra Bombicz and Edwin Weber*

A calix[4] arene with a single laterally-substituted carboxylic acid group is studied, and the conformational behaviour in solution and crystal structures of the unsolvated and solvated species determined.





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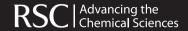


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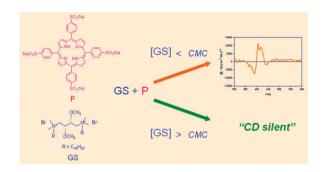


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Propagation of chirality from gemini surfactants to porphyrin/surfactant heteroaggregates: transcription of the stereochemical information into an organizational feature

Zoubir El-Hachemi, Giovanna Mancini,* Josep M. Ribó and Alessandro Sorrenti

The chirality of a gemini surfactant controls the chiral morphology of porphyrins organized in H-type aggregates formed below the critical micellar concentration of the surfactant.

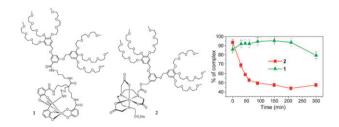


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Synthesis and characterization of a highly stable dendritic catechol-tripod bearing technetium-99m

Annabelle Bertin, Anne-Isabelle Michou-Gallani, Jérôme Steibel, Jean-Louis Gallani and Delphine Felder-Flesch*

A dendritic ^{99m}Tc ligand 1 derived from a pre-organized tripodal tris-catecholamide exhibits a kinetic stability by far more important than its corresponding diethylenetriamine pentaacetic acid homologue 2.

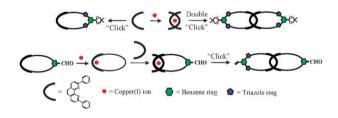


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Introduction of useful peripheral functional groups on [2]catenanes by combining Cu(1) template synthesis with "click" chemistry

Jackson D. Megiatto, Jr.* and David I. Schuster*

Two protocols based on Cu(I) template synthesis and "click" reactions for the synthesis of functionalized macrocycles and [2]catenanes are described. The introduction of peripheral functional groups into the catenane structure opens up possibilities of using these materials as building blocks for preparation of even more complex structures.

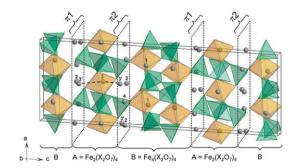


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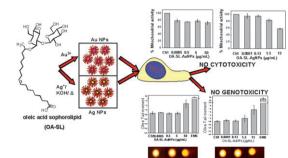
Crystal structures and sodium/silver distributions within the ionic conductors Na₅Ag₂Fe₃(As₂O₇)₄ and Na₂Ag₅Fe₃(P₂O₇)₄

Eric Quarez,* Olivier Mentré, Karim Djellab and Christian Masquelier

Crystal structures of new Na₅Ag₂Fe₃(As₂O₇)₄ and $Na_2Ag_5Fe_3(P_2O_7)_4$ compounds are reported.



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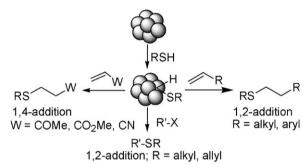


Cytotoxic and genotoxic assessment of glycolipid-reduced and -capped gold and silver nanoparticles

Sanjay Singh, V. D'Britto, A. A. Prabhune, C. V. Ramana, Alok Dhawan* and B. L. V. Prasad*

No cytotoxicity and genotoxicity: sophorolipid (a class of glycolipid)-conjugated silver and gold nanoparticles do not show any cytotoxic and genotoxic effects up to $100~\mu M$ metal concentrations.

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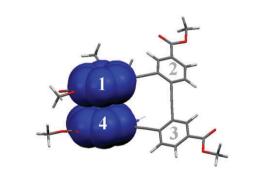


Silica nanoparticles as a reusable catalyst: a straightforward route for the synthesis of thioethers, thioesters, vinyl thioethers and thio-Michael adducts under neutral reaction conditions

Subhash Banerjee,* Jayanta Das, Richard P. Alvarez and Swadeshmukul Santra*

A simple and straightforward route for the synthesis of thioethers, thioesters, vinyl thioethers and thio-Michael adducts has been demonstrated using free silica nanoparticles as a reusable catalyst *via* the 1,2-addition of thiols to alkenes, alkynes and alkyl/acyl halides, and the 1,4-addition of thiols to conjugated alkenes at room temperature.

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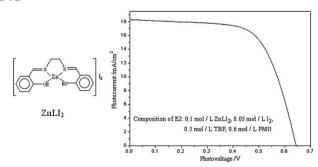


Apolar *ortho*-phenylene ethynylene oligomers: conformational ordering without intermolecular aggregation

Jing Jiang, Morris M. Slutsky, Ticora V. Jones and Gregory N. Tew*

Non-polar alkoxy substituted *ortho*-phenylene ethynylene (*o*-PE) oligomers with lengths up to nine units have been shown to adopt helical conformations in heptane by NMR and CD spectroscopy, while chloroform promotes extended conformations.

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Efficient electrolyte of N,N'-bis(salicylidene)ethylenediamine zinc(II) iodide in dye-sensitized solar cells

Shuming Yang,* Huizhi Kou, Hongjun Wang, Ke Cheng and Jichao Wang

N,N'-Bis(salicylidene)ethylenediamine zinc(II) iodide (ZnLI₂) was synthesized and applied as an efficient electrolyte in dye-sensitized solar cells, and found to have a photoelectric conversion efficiency of 7.75% with electrolyte E2 under 100 mW cm⁻² irradiation.

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Conjugated ethynylene-fluorene polymers with electro-donating TTF as pendant groups: Synthesis, electrochemical and spectroscopic properties

Xuechao Zhang, Chengyun Wang,* Guoqiao Lai, Lei Zhang and Yongjia Shen*

A series of conjugated ethynylene-fluorene polymers with TTF as pendant groups were synthesized. These polymers exhibited good solubility and improving conductivity up to about $1-3 \times 10^{-3} \,\mathrm{S \, cm^{-1}}$.

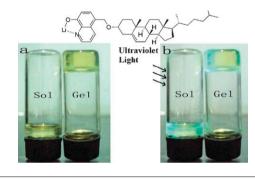
$$\begin{array}{c} \text{TTF-}(H_2C)_6 & (CH_2)_6 & \text{TTF} \\ \hline \\ \text{Aryl=} & \begin{array}{c} \\ \\ \end{array} & \begin{array}{c} \\ \\ \end{array}$$

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Enhanced photoluminescence and the self-assembled fibrillar nanostructure of 5-(cholesteryloxy)methyl-8-hydroxyquinoline lithium in a gel state

Sheng Kong, Lixin Xiao,* Zhijian Chen, Xingzhong Yan, Bo Qu, Shufeng Wang and Qihuang Gong*

A soluble, highly efficient, fluorescent, organometallic gelator, LiChQ, was synthesized through the modification of LiQ with cholesterol.

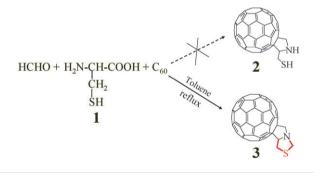


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One-pot synthesis of new thio-derivatives of C_{60} with the unexpected formation of a thiazolidine-fulleropyrrolidine

Chuanbao Chen, Xiaofang Li and Shangfeng Yang*

One-pot Prato reactions of C₆₀ with amino acids and aldehydes afford five new fullerene derivatives via 1,3-dipolar cycloaddition. These include the thiazolidine-fulleropyrrolidine 3, the formation of which relies on the presence of the active S-H hydrogen in 1.

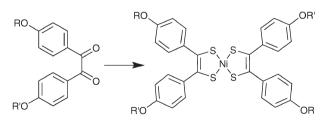




Synthesis and preliminary physical properties of new neutral tetraalkoxy-substituted nickel bis(1,2-dithiolene) complexes

Thanh-Tuan Bui, Bénédicte Garreau-de Bonneval and Kathleen I. Moineau-Chane Ching*

Nineteen neutral nickel bisdiphenylethenedithiolene complexes [Ni(dpedt)₂], including seventeen new compounds, were synthesized and characterized by a new short, efficient and multigram-scale synthetic method.



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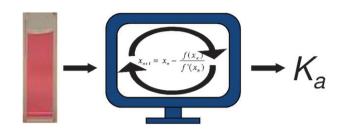
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Algorithms for the determination of binding constants and enantiomeric excess in complex host: guest equilibria using optical measurements

Amanda E. Hargrove, Zhenlin Zhong, Jonathan L. Sessler* and Eric V. Anslyn*

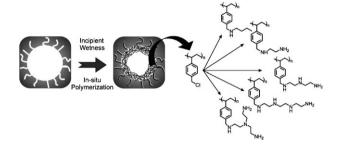
An iterative method using commercial software that allows for the rigorous determination of binding constants in a variety of systems, including 1:2 complexes, indicator displacement assays, and enantioselective indicator displacement assays has been developed.

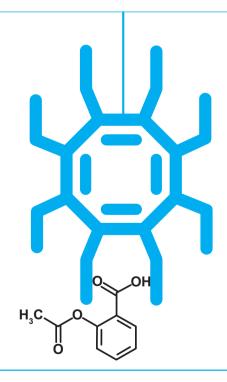


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Insights into pore surface modification of mesoporous polymer-silica composites: introduction of reactive amines

Rémy Guillet-Nicolas, Louis Marcoux and Freddy Kleitz* Tailored mesoporous amine-functionalized polymer-silica composites are synthesized using a two-step mesopore surface-confined polymerization technique.





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