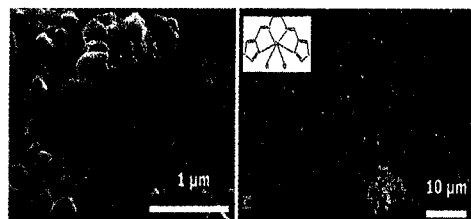


MTPP(Ph)₃X₅
 M = 2H, Ni(II); X = Cl
 M = Ni(II); X = CN

Crystal structures of unsymmetrically mixed β -pyrrole substituted nickel(II)-*meso*-tetraphenylporphyrins

Bhyrappa Puttaiah, Velkannan Veerapandian and Sarangi Ujwal Kumar 1047–1055

Crystal structures of solvated 2,3,12,13,17-penta(chloro or cyano)-5,7,8,10,15,18,20-heptaphenylporphyrin H₂TPP(Ph)₃(Cl)₅, and their Ni(II) complexes, NiTPP(Ph)₃(Cl)₅ and NiTPP(Ph)₃(CN)₅ were determined by single crystal XRD. They revealed nonplanar conformation of the macrocycle ($\Delta C_b > \pm 0.9 \text{ \AA}$). The structures were examined by normal-coordinate structural decomposition and Hirshfeld surface analyses.



Copper(II) Schiff base complexes and their mixed thin layers with ZnO nanoparticles

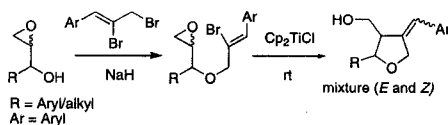
Magdalena Barwiolek, Robert Szczęśny and Edward Szyk . . . 1057–1066

New copper(II) complexes with Schiff bases obtained from ethylenediamine were structurally and spectroscopically characterized. Thin layers of Cu(II) complexes were deposited on Si(111) or ZnO/Si(111) by a spin coating method. The Cu(II) layers exhibited fluorescence bands between 462 and 503 nm. In the Cu(II)complex/ZnO/Si layers, quenching of the emission band from ZnO at 440 nm ($\lambda_{ex}=330 \text{ nm}$) was noted.

Titanocene(III) chloride mediated radical induced addition-elimination route to the synthesis of racemic and optically active trisubstituted tetrahydrofurans: Formal synthesis of magnofargesin and 7'-epimagnofargesin

P Chakraborty, S K Mandal and S C Roy 1067–1079

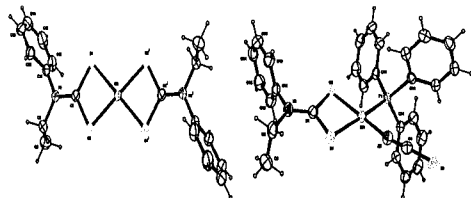
Titanocene(III) Chloride mediated, radical induced synthesis of 4-benzylidene substituted tetrahydrofuran, a typical lignan skeleton, has been accomplished in good yield through addition-elimination route in racemic as well as in optically active forms. The method has been applied to the synthesis of furano lignans, magnofargesin and 7'-epimagnofargesin in optically active forms.



Synthesis, crystal structure, thermal and theoretical studies of bis(*N*-ethyl-*N*-phenyldithiocarbamato) Ni(II) and (*N*-ethyl-*N*-phenyldithiocarbamato) (isothiocyanato) (triphenylphosphine) Ni(II)

Damian C Onwudiwe, Mwadham M Kabanda, Eno E Ebenso and Eric Hosten 1081–1093

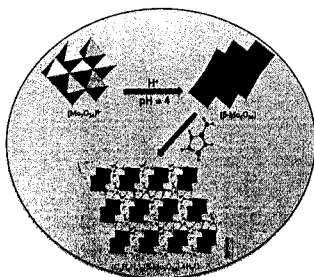
Ni(II) complexes of dithiocarbamate were synthesized and characterized. The optimized geometry and the electronic analysis of the type of bonding within the complex structures were performed using methods based on the density functional theory and atom in molecule (AIM) analysis method.



Assembly of organic moiety with metal-oxide cluster to generate a new three dimensional supramolecular/hydrogen bonded network based on isopolymolybdate

Donia Zammel, Ichraf Nagazi and Amor Haddad 1141–1148

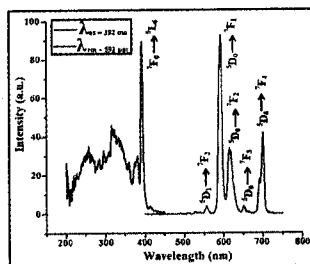
A new organic–inorganic hybrid material was prepared from ammonium *hepta*-molybdate in acidic medium by addition of 1, 2, 4-triazol-3-amine to obtain an *octa*-molybdate formulated as $(C_2H_6N_4)_2 [\beta-Mo_8O_{26}].4H_2O$. The compound was characterized by single crystal X-ray diffraction method, IR spectroscopy, UV-Vis absorption, thermogravimetric analysis and cyclic voltammetry.



Synthesis and characterization of bi-functional magneto-luminescent $Fe_3O_4@SiO_2@NaLuF_4:Eu^{3+}$ hybrid core/shell nanospheres

Jigmet Ladol, Heena Khajuria, Haq Nawaz Sheikh and Yugal Khajuria 1149–1155

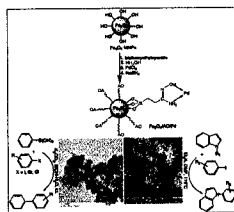
Bi-functional magneto luminescent $Fe_3O_4@SiO_2@NaLuF_4:Eu^{3+}$ hybrid core/shell nanospheres synthesized *via* step-wise method is reported. The Fe_3O_4 magnetic core exhibits super-paramagnetic behavior at room temperature whereas europium-doped sodium lutetium fluoride ($NaLuF_4:Eu^{3+}$) shell induces highly efficient luminescent intensity with average lifetime value of 6.235 ns.



Pd immobilized on modified magnetic Fe_3O_4 nanoparticles: Magnetically recoverable and reusable Pd nanocatalyst for Suzuki-Miyaura coupling reactions and Ullmann-type *N*-arylation of indoles

Ramin Ghorbani-Vaghei, Saba Hemmati and Malak Hekmati . . . 1157–1162

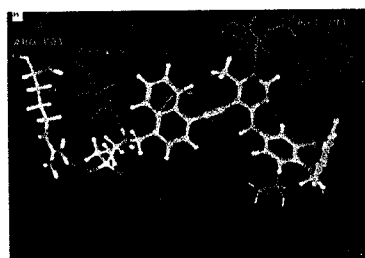
Pd supported on amidoxime (AO)-functionalized Fe_3O_4 nanoparticles ($Fe_3O_4/AO/Pd$) showed high catalytic activity in Suzuki and Ullmann coupling reaction.



Molecular docking, MM/GBSA and 3D-QSAR studies on EGFR inhibitors

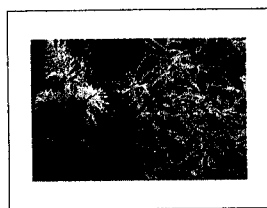
Raju Bathini, Sree Kanth Sivan, Sabiha Fatima and Vijjulatha Manga 1163–1173

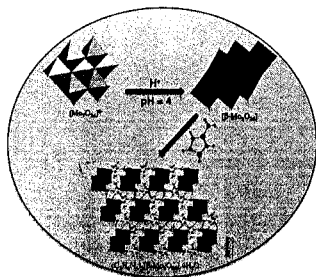
Epidermal growth factor receptor (EGFR) is the first growth factor receptor proposed as a target for cancer therapy. An integrated computational protocol using molecular docking and 3D QSAR were performed using the CoMFA and CoMSIA methods. Derived models showed good statistical reliability that is evident from their r^2 , q^2_{loo} values. Information obtained from 3D QSAR model was applied for optimization of lead molecules and to design novel potential inhibitors.



Dockpose of newly designed molecule showing hydrogen bond interaction with active site amino acids along with steric regions

Cover picture: Cu(I)-catalyzed Intramolecular Photocycloaddition to Oxacyclobutapentalene. For details, see the paper by Ritabrata Datta *et al.* (pp. 1019–1023)

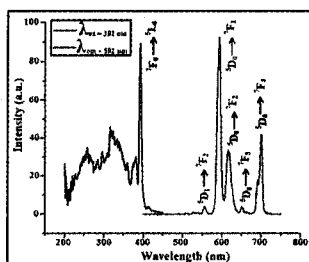




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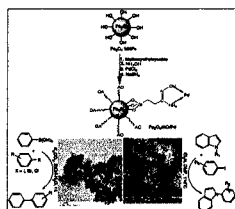
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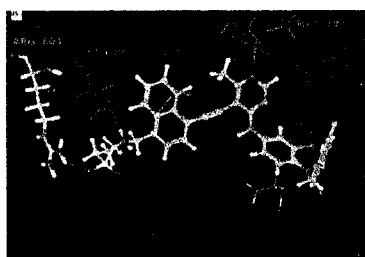
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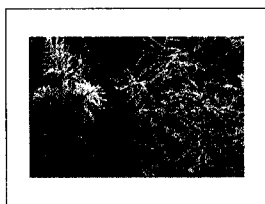


Dockpose of newly designed molecule showing hydrogen bond interaction with active site amino acids along with sitemap regions

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Cover picture: Cu(I)-catalyzed Intramolecular Photocycloaddition to Oxacyclobutapentalene. For details, see the paper by Ritabrata Datta *et al.* (pp. 1019–1023)

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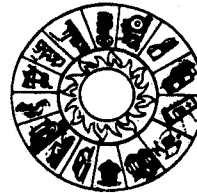
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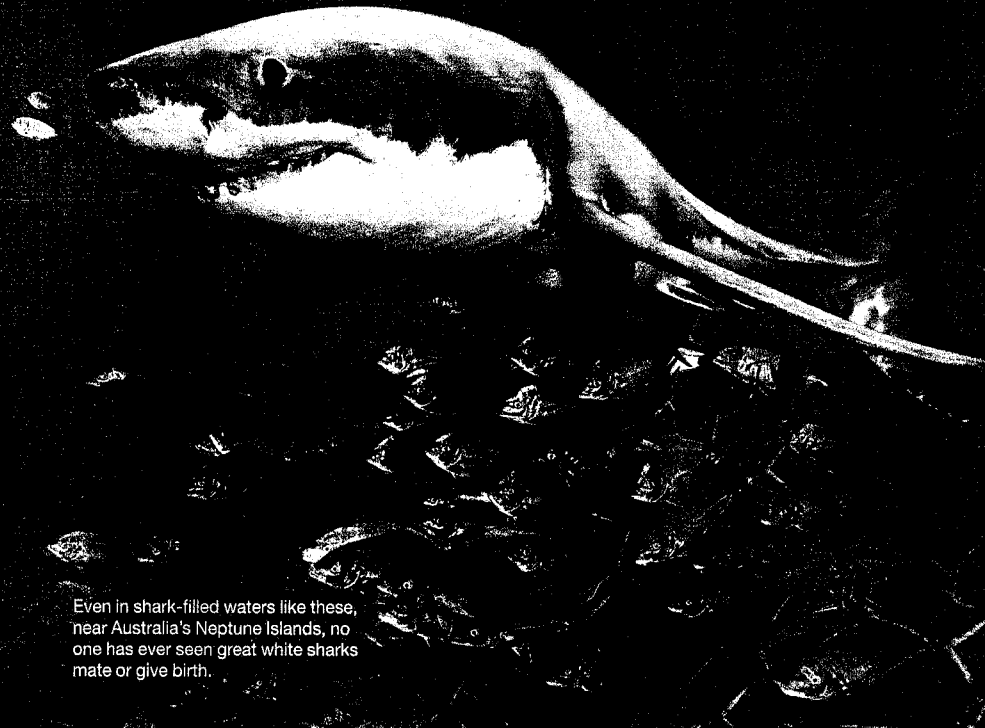
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Even in shark-filled waters like these, near Australia's Neptune Islands, no one has ever seen great white sharks mate or give birth.

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Great White Mystery

They are the world's most famous sharks—yet we know so little about them.

By Erik Vance Photographs by Brian Skerry

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The Battle for Virunga

At one of the world's most dangerous parks, survival depends upon making peace with desperate, discontented neighbors.

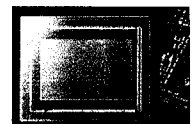
By Robert Draper
Photographs by Brent Stirton

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Greece, Gods, and the Beyond

Ancient Greeks believed that gods played a role in all life, from the underworld to realms above.

By Caroline Alexander
Photographs by
Vincent J. Musi and David Coventry

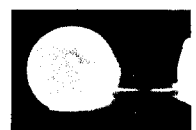


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After more than 20 years abroad, a
photographer explores his own country.
Story and Photographs by David Guttentfelder

On the Cover Fingerprint analysis, which investigators have used to help solve crimes since the late 1800s, is now being reevaluated, along with other forensic science practices. Photo by ar-chil/Getty Images

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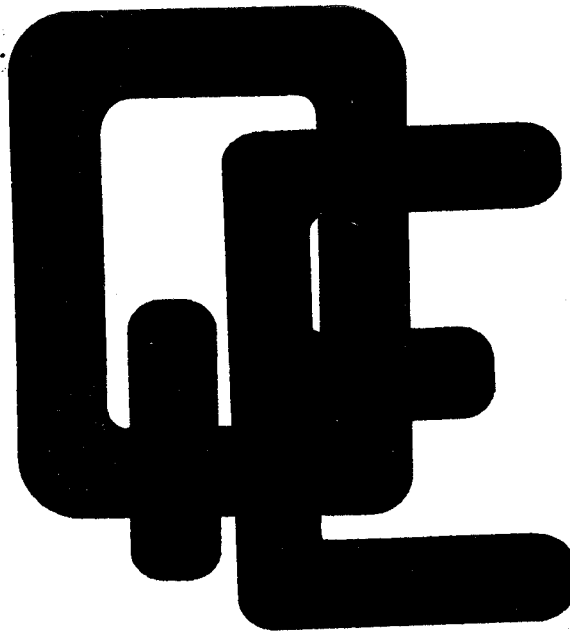
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