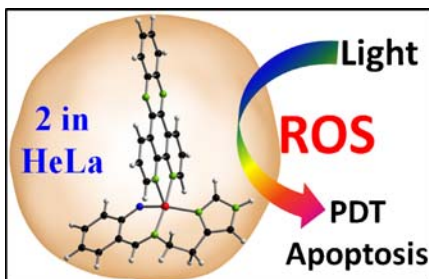


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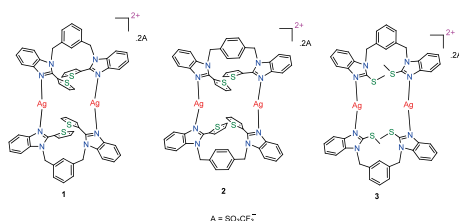
Regular Articles



Photocytotoxic ternary copper(II) complexes of histamine Schiff base and pyridyl ligands

Samya Banerjee, Akanksha Dixit, K Sessa Maheswaramma, Basudev Maity, Sanjoy Mukherjee, Arun Kumar, Anjali A Karande and Akhil R Chakravarty 165–175

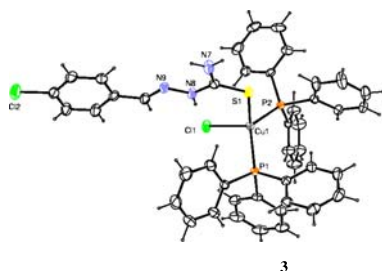
Schiff base copper(II) complex of dipyrrophenazine shows remarkable photocytotoxic effect in HeLa cells in visible light (400-700 nm) with reduced dark toxicity via apoptotic pathway. The complex intercalatively binds to ct-DNA, exhibits moderate chemical nuclease activity but excellent DNA photocleavage activity in red light of 705 nm forming $\bullet\text{OH}$ radicals.



Silver(I) based dinuclear metallacycles with free thiophenyl/thiomethyl units

Sarita Yadav, Deepak Gupta and Malaichamy Sathiyendiran 177–184

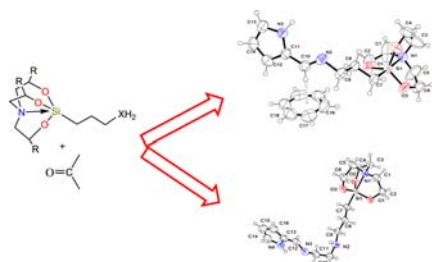
A new type of silver metallacycles with covalently attached free thiophenyl/thiomethyl units was synthesized using $\text{AgOS(O)}_2\text{CF}_3$ and ditopic ligands and characterized by using crystallographic and spectroscopic techniques.



Synthesis and crystal structure of [chlorobis(triphenylphosphino) (p-chlorobenzaldehyde thiosemicarbazone)] copper(I) complex

Ashiq Khan, Poonam Sharma, Rajnikant, Vivek K Gupta, Naresh Padha and Rekha Sharma 185–191

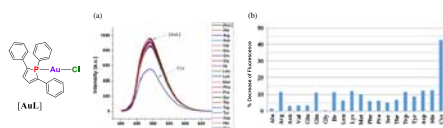
p-Chlorobenzaldehyde thiosemicarbazone formed tetrahedral monomeric complex 3 with copper(I) chloride in the presence of triphenylphosphine. The intermolecular H-bonding, $\text{Cl} \cdots \text{HC}_{\text{ph}}$, 2.733 Å and π interactions, $\{\text{CH}_{\text{ph}} \cdots \pi$, 2.796; 2.776 Å} in this complex led to the formation of 1D chain.



Schiff base functionalized Organopropylsilatranes: Synthesis and structural characterization

Gurjaspreet Singh, Promila, Amandeep Saroa, Jandeep Singh, Raj Pal Sharma and V Ferretti 193–200

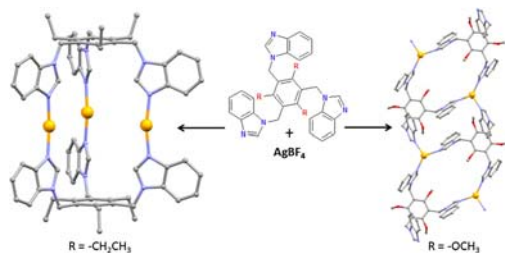
Synthesis of Schiff bases linked to organopropylsilatranes was performed by condensation reaction of post-functionalized silatranes with two different aldehydes viz. pyrrole-2-carboxaldehyde and 2-hydroxy-1-naphthaldehyde. The resulting Schiff base substituted silatranes were well characterized by elemental analysis, spectroscopic studies (IR, ^1H , ^{13}C) NMR, MS and by single crystal X-ray diffraction analysis).



Chloro(triphenylphosphole)gold(I) - A selective Chemosensor for Cysteine

Maruthai Kumaravel and Maravanji S Balakrishna 201–206

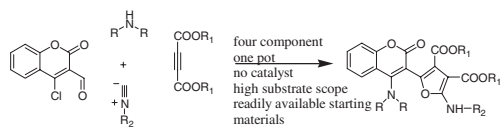
Photophysical studies of luminescent gold complex of triphenylphosphole have been described.



Conformation driven complexation of two analogous benzimidazole based tripodal ligands with Ag(I) resulting in a trigonal prism and a coordination polymer

Suman Bhattacharya and Binoy K Saha 207–216

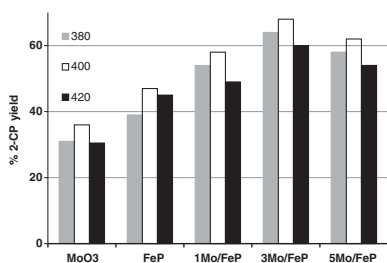
Complexation of silver(I) tetrafluoroborate with two analogous benzimidazole based tripodal ligands namely **1-Et** and **1-OMe**, led to the formation of a zero dimensional trigonal prism in case of the former, whereas a one dimensional coordination polymeric ladder in case of the latter. The complexation reactions in respective cases were found to depend on the conformation of the ligating center of the two ligands.



One-pot four component synthesis of novel 3-furyl coumarin derivatives

Venkata Prasad Jalli, Suvratha Krishnamurthy, Tetsuji Moriguchi and Akihiko Tsuge 217–226

Synthesis of 3-furyl coumarin derivatives have been achieved by reaction of 4-chloro-3-formylcoumarin, secondary amines, dialkyl acetylenedicarboxylates and diversely substituted isocyanides using four component, one-pot reaction.

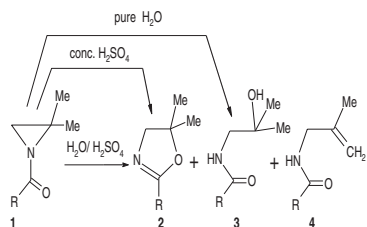


Amoxidation of 2-methyl pyrazine to 2-cyano pyrazine on MoO₃/FePO₄ catalysts

Nagaraju Pasupulety, Hafedh Driss, Yahia Abobakor Alhamed, Abdulrahim Ahmed Alzahrani, Muhammad A Daous, Lachezar Petrov, N Lingaiah and P S Sai Prasad 227–234

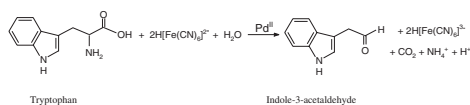
The influence of a small amount of Mo=O (1, 3 and 5 wt.% MoO₃) impregnated on FePO₄ and its resultant effect on the acidity was studied for the amoxidation of 2-methyl pyrazine (2-MP) to 2-cyano pyrazine (2-CP) in the temperature range of 380-420°C.

Experimental and theoretical rearrangement of N-acyl-2,2-dimethylaziridines in acidic medium



Madiha Kamoun Mhiri, Firas Aboumessaad, Mohamed Lotfi Efrif, Youssef Arfaoui and Néji Besbes 235–245

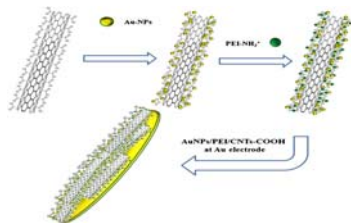
The acidic aqueous solutions of the N-acyl-2,2-dimethylaziridines **1** lead to a mixture of oxazolines **2**, amidoalcohols **3** and methallylamides **4**. The mechanism proposed to explain the formation of products **2-4** have been confirmed by the quantum chemical calculations using the DFT/B3LYP method and 6-311++G(2d,2p) basis set.



Palladium(II)-catalyzed oxidation of L-tryptophan by hexacyanoferrate(III) in perchloric acid medium: a kinetic and mechanistic approach

Ahmed Fawzy, 247–256

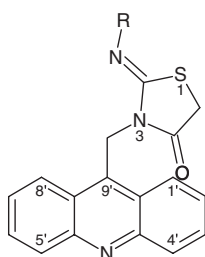
Palladium(II)-catalyzed oxidation of L-tryptophan by hexacyanoferrate(III) in aqueous perchloric acid medium has been investigated. The effect of temperature on the reaction rate has been studied and the activation parameters have been evaluated and discussed. The final oxidation products are identified as indole-3-acetaldehyde, ammonium ion and carbon dioxide.



Acriflavine immobilized onto polyethyleneimine-wrapped carbon nanotubes/gold nanoparticles as an electrochemical sensing platform

Azadeh Azadbakht and Amirreza Abbasi. 257–268

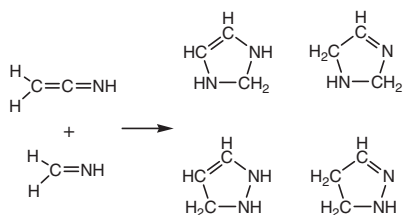
Polyethyleneimine wrapped, multi-walled carbon nanotubes functionalized with a carboxylic acid group and gold nanoparticles has been utilized as a platform to immobilize poly(acriflavine) and used as electrochemical sensor for H_2O_2 .



Unexpected regioselective formation and DNA binding of new 3-(acridin-9-yl)methyl-2-iminothiazolidin-4-ones

Ján Imrich, Danica Sabolová, Mária Vilková and Júlia Kudláčová. 269–277

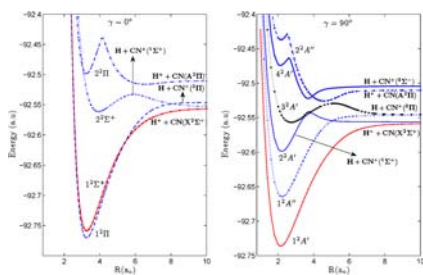
New DNA-binders 3-(acridin-9-yl)methyl-2-R-imino-1,3-thiazolidin-4-ones were regioselectively synthesized from unstable (acridin-9-yl)methyl thioureas and methyl bromoacetate (MBA) or bromoacetyl bromide (BAB) by a mechanism involving a transient spiro 9,10-dihydroacridine intermediate.



Theoretical insights into the cycloaddition reaction mechanism between ketenimine and methyleneimine: An alternative approach to the formation of pyrazole and imidazole

Nana Wang, Xiaojun Tan, Weihua Wang, Fangfang Wang and Ping Li. 279–285

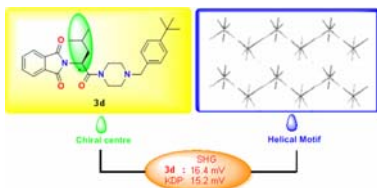
The cycloaddition reaction mechanism between interstellar molecules, ketenimine and methyleneimine, has been systematically investigated theoretically. The products of this reaction are pyrazole and imidazole compounds, respectively.



Ab initio adiabatic and quasidiabatic potential energy surfaces of $H^+ + CN$ system

Bhargava Anusuri and Sanjay Kumar. 287–296

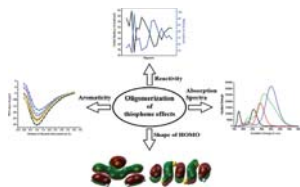
We present *ab initio* three dimensional potential energy surfaces for $H^+ + CN$ system. The calculations were performed at the internally contracted multi-reference configuration interaction (*ic*MRCI) level of theory using Dunning's correlation consistent polarized valence triple zeta (*cc*-pVTZ) basis set. Adiabatic and quasidiabatic surfaces were computed for ground and first excited electronic states for the collinear and perpendicular approaches of H^+ . Nonadiabatic effects arising from radial coupling have been analyzed in terms of nonadiabatic coupling matrix elements (NACME) and coupling potentials.



Functionalized organic frameworks explored as second order NLO agents

Anil K Singh, Brijesh Rathi, Volodymyr V Medvediev, Oleg V Shishkin, Vijay Bahadur, Taruna Singh, Brajendra K Singh, N Vijayan, V Balachandran and Nikolay Yu Gorobets. 297–309

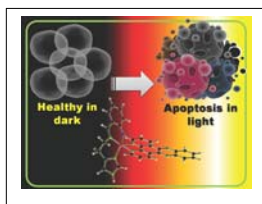
New chiral phthalimides possessing terminal arylpiperazines have been studied for their solid-state properties. The second order NLO response of all the listed phthalimides was substantiated with the aid of computational study and crystal engineering approach.



Does oligomerization in fused thiophene affect reactivity and aromaticity?

Siddhartha Kr Purkayastha and Pradip Kr Bhattacharyya. . . 311–324

Reactivity and aromatic character of thiophene is influenced by oligomerization.



Cover picture: Light-activated Metal-based Anticancer Agents. For details, see the paper by Samya Banerjee *et al.* (pp. 165–175)