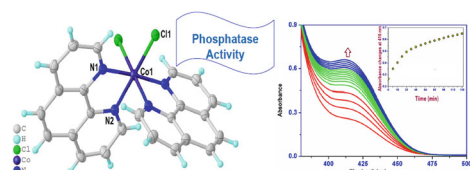


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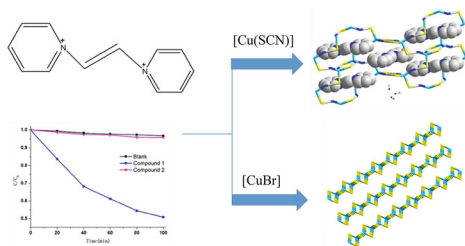


Synthesis and phosphatase activity of a Cobalt(II) phenanthroline complex

Mamoni Garai, Dhananjay Dey, Hare Ram Yadav, Milan Maji, Angshuman Roy Choudhury and Bhaskar Biswas 1513–1520

The cobalt(II) complex of phenanthroline exhibits good catalytic activity towards 4-nitrophenylphosphate (PNPP) as a standard substrate in aqueous DMF medium with k_{cat} value of $3.78 \times 10^2 \text{h}^{-1}$

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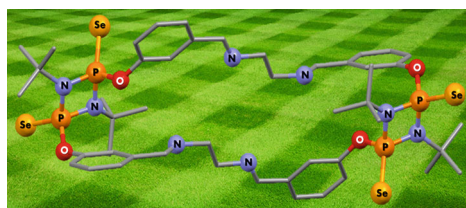


Two new supramolecular compounds induced by novel vinylpyridine cationic templates: synthesis, structures and enhanced photocatalytic properties

Min Xiao, Su-Min Li and Yun-Yin Niu 1521–1530

Two novel complexes $\{(pepy)[Cu_2(SCN)_4]\}_n$ and $\{(pepy)[Cu_2(Br_4)]\}_n$ [Pepy=1-2-(Pyridinium-1-yl)-1-ethenyl] pyridinium] based on vinylpyridinium cation and cuprous salts have been synthesized. They exhibited diverse structures and good photocatalytic properties.

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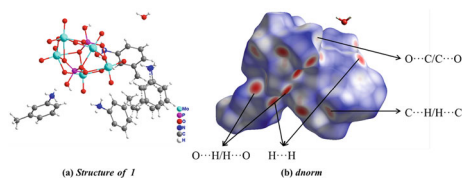


Macrocyclic cyclodiphosphazane $\{[P(\mu\text{-}^i\text{BuN})_2](O - m - C_6H_4 CHNCH_2)_2\}_2$: synthesis of chalcogen derivatives and gold(I) complex

Vitthalrao S Kashid, Joel T Mague, and Maravanji S Balakrishna 1531–1537

The synthesis of chalcogenides and gold complex of a Schiff base appended cyclodiphosphazane containing macrocycle $\{[P(\mu\text{-}^i\text{BuN})_2](O - m - C_6H_4 CHNCH_2)_2\}_2$ is described.

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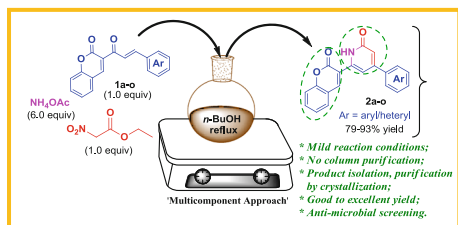


Synthesis, characterization, Hirshfeld surface and theoretical properties of $(C_7H_{10}N)_4[H_2P_2Mo_5O_{23}] \cdot H_2O$

Ali Harchani, Monika Kučeráková, Michal Dušek, and Amor Haddad 1539–1547

The title compound $(C_7H_{10}N)_4[H_2P_2Mo_5O_{23}] \cdot H_2O$ was synthesized and characterized by IR and UV spectroscopy, and its structure was solved by single crystal X-ray diffraction. The presence of the Mo, P, O, C and N atoms was confirmed by EDS analysis. The Hirshfeld surface analysis was performed to elucidate non-bonding interactions and theoretical properties were calculated.

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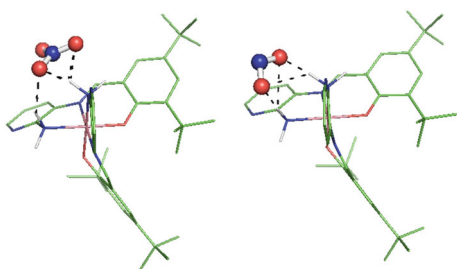


Expedient synthesis of coumarin-pyridone conjugates molecules and their anti-microbial evaluation

Rajni Khajuria, Sheena Mahajan, Ambica and Kamal K Kapoor 1549–1557

Expedient synthesis of coumarin-pyridone conjugate molecules has been reported *via* one-pot, three-component reaction between (*E*)-3-(3-arylacryloyl)-2*H*-chromen-2-ones, ethyl 2-nitroacetate and ammonium acetate. Anti-microbial activity of these compounds was evaluated and the results indicated that some of the compounds exhibited mild anti-bacterial activity and good inhibitory potential against the tested fungal organisms.

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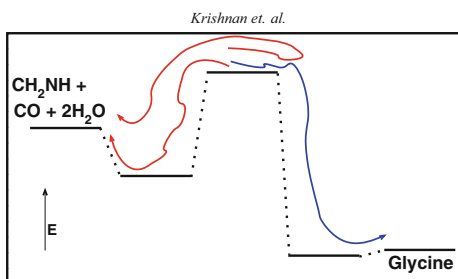


A new Co(III) complex of Schiff base derivative for electrochemical recognition of nitrite anion

Hakan Yilmaz, Abdulkadir Kocak, Maowulidan Dilimulati, Yunus Zorlu and Muberra Andac 1559–1569

An octahedral Co(III) complex of the salphen-type Schiff base, (*E*)-2-([(2-aminopyridin-3-yl)imino]methyl)-4,6-di-*tert*-butylphenol, was synthesized, characterized and analyzed for its electrochemical anion recognition property through reversible anion exchange mechanism.

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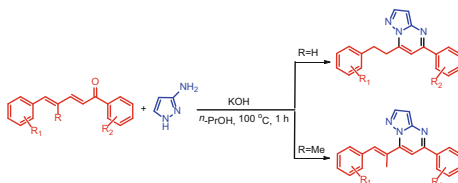


Classical dynamics simulations of interstellar glycine formation via $\text{CH}_2 = \text{NH} + \text{CO} + \text{H}_2\text{O}$ reaction

Yogeshwaran Krishnan, Allen Vincent and Manikandan Paranjothy 1571–1577

Glycine formation in the interstellar media *via* the $\text{CH}_2 = \text{NH} + \text{CO} + \text{H}_2\text{O}$ reaction was investigated by classical chemical dynamics simulations. This reaction has a large barrier which reduces in presence of additional water molecules. Our simulations indicate that the proposed catalytic effect by the additional water molecules may not be a classical effect.

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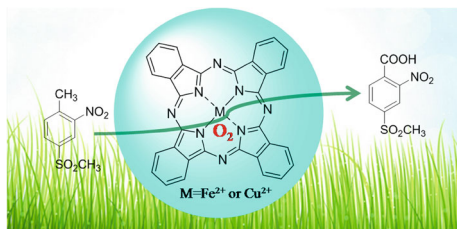


Synthesis of 7-arylethyl-5-arylpyrazolo [1,5-*a*] pyrimidines through an aza-Michael addition/nucleophilic addition/1,3-hydrogen transfer cascade

Zheng Li, Demeng Xie, Jiaojiao He, Yan Du and Jingya Yang 1579–1586

Arylethyl-5-arylpyrazolo [1,5-*a*]pyrimidines were efficiently synthesized by the reactions of 4-unsubstituted dienones with pyrazole-3-amine. In contrast, 7-arylethylene-5-arylpyrazolo [1,5-*a*] pyrimidines could be afforded by the reactions of 4-substituted dienones with pyrazole-3-amine.

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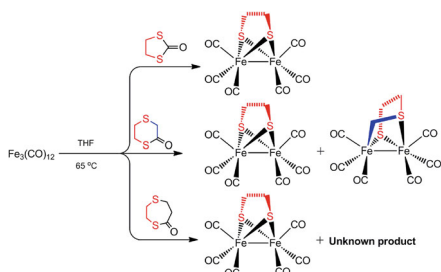


Iron(II) and copper(II) phthalocyanine-catalyzed synthesis of 2-nitro-4-methylsulfonylbenzoic acid under mild conditions

Cheng Huang, Rui Liu, Caiting Zhang, Qipeng Cheng and Hongjun Zhu1587–1594

A novel method to produce 2-nitro-4-methylsulfonylbenzoic acid (NMSBA) from the oxidation of 2-nitro-4-methylsulfonyltoluene (NMST) by oxygen catalyzed by iron(II) phthalocyanine (FePc) and copper(II) phthalocyanine (CuPc) has been developed. The reaction parameters and mechanism were studied. The catalytic system will be readily applicable to large-scale production of NMSBA.

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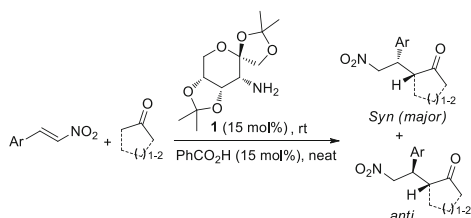


Reaction of three cyclic thioester ligands with triiron dodecacarbonyl and possible reaction mechanisms

Zhiyin Xiao, Yongli Wang, Xueyuan Chen, Jiao Long, and Zhenhong Wei1595–1601

Reaction of cyclic thioester ligands with triiron dodecacarbonyl leads to scission of C-S (C) bond which is initiated by the coordination of the S atom to the Fe atom. The larger the ring size of the ligand, the more diverse are the bond cleavages.

Rapid Communication

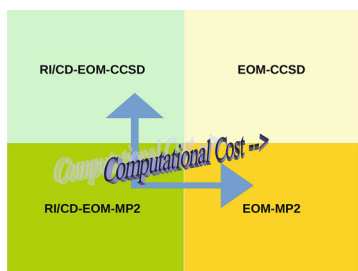


Enantioselective aminocatalysis: Michael addition of unactivated ketones to nitroolefins catalyzed by D-fructose derived monofunctional primary amine

Khiangte Vanlaldinpuia, Porag Bora, Grace Basumatary, Rahul Mohanta and Ghanashyam Bez1603–1610

Monofunctional primary amine is used for the first time as catalyst for stereoselective Michael addition reaction of different ketones to nitro olefins to synthesize γ -nitro carbonyl compounds.

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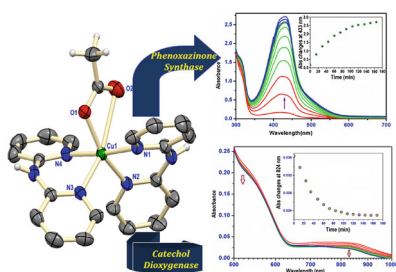


Resolution of the Identity and Cholesky Representation of EOM-MP2 Approximation: Implementation, Accuracy and Efficiency

Dinesh Kumar, Achintya Kumar Dutta and Prashant Uday Manohar1611–1626

We present RI/CD implementation on EOM-MP2 method for computing IP, EA, EE and SF target electronic states of molecules. The RI/CD implementation results in speed-up in computational time and reduction in storage requirements without much compromise on accuracy, thereby widening the applicability of the method to molecules of bigger computational size.

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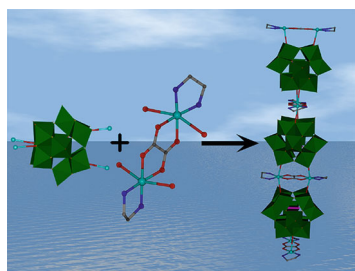


Catalytic aspects of a copper(II) complex: biological oxidase to oxygenase activity

Biswajit Chowdhury, Milan Maji and Bhaskar Biswas. . . . 1627–1637

The mononuclear copper complex having unusual hexa coordination geometry exhibits significant catalytic efficiency, $k_{\text{cat}}/K_{\text{M}}(\text{h}^{-1}) = 6.17 \times 10^5$ towards oxidation of 2-aminophenol which predominantly produced extradiol cleavage products at a rate, $k_{\text{obs}} = 1.09 \times 10^{-3} \text{ min}^{-1}$, upon addition of 3,5-DTBC in presence of molecular oxygen.

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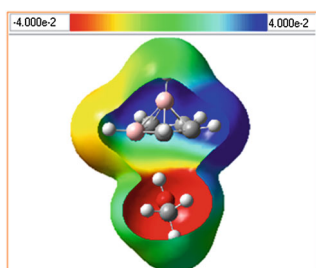


Two hybrids based on Keggin polyoxometalates and dinuclear copper(II) complexes: syntheses, structures and electrocatalytic properties

Yan Hou, Ying Niu, Chunjing Zhang, Haijun Pang and Huiyuan Ma. 1639–1645

Two new hybrids based on polyoxoanions and dinuclear copper complexes have been synthesized and characterized. The results of electrocatalytic experiments indicate that the hybrid-based electrode possesses high catalytic efficiency and selectivity towards reduction of H_2O_2

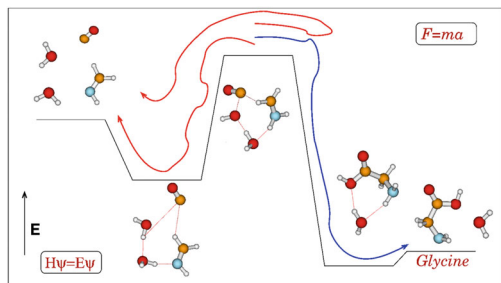
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The noncovalent complexes of nido- $\text{C}_4\text{B}_2\text{H}_6$ with H_2O , CH_3OH and NH_3 Lewis bases: A Theoretical study

Nahid Zare and Abedien Zabardasti 1647–1657

There are various orientations for $\text{C}_4\text{B}_2\text{H}_6$ to interact with both Lewis acids and bases. According to the minimal molecular electrostatic potential (MEP) calculations, the highest electron density is concentrated on the B-H bonds while the lowest one is on the C-H bonds. On the other hand, the basal plane of the $\text{C}_4\text{B}_2\text{H}_6$ has both abilities, in a way that the most stable complex is achieved when the basal plane interacts with the target molecules.



Cover picture: Dynamics of Interstellar Glycine Formation.
For details, see the paper by Yogeshwaran Krishnan *et al.* (pp. 1571–1577)