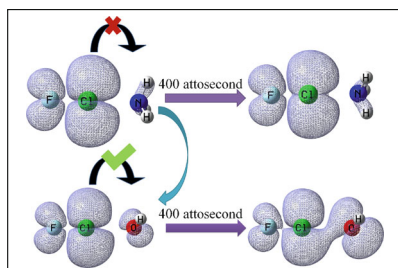


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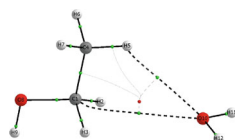
Regular Articles



On the Attosecond charge migration in $\text{Cl}\cdots\text{N}$, $\text{Cl}\cdots\text{O}$, $\text{Br}\cdots\text{N}$ and $\text{Br}\cdots\text{O}$ Halogen-bonded clusters: Effect of donor, acceptor, vibration, rotation, and electron correlation

Sankhabrata Chandra, Mohammed Musthafa Iqbal and Atanu Bhattacharya 1175–1189

The attosecond charge migration dynamics through $\text{Cl}\cdots\text{N}$, $\text{Cl}\cdots\text{O}$, $\text{Br}\cdots\text{N}$, and $\text{Br}\cdots\text{O}$ halogen bonds depends on strength of electron correlation, donor and acceptor, the energy difference (ΔE) between two stationary cationic orbitals (LUMO- β and HOMO- β) involved in electronic superposition, vibration and rotation.

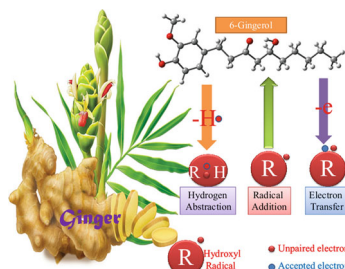


O...C bond (carbon bond) and C-H...O bond (hydrogen bond) in $\text{C}_2\text{H}_5\text{OH}\cdots\text{H}_2\text{O}$ Complex

$\text{C}_2\text{H}_5\text{OH}\cdots\text{HX}$ ($\text{X}=\text{OH}$, SH , F) interactions: Is there a carbon bond?

Amar Bahadur G C and Rajendra Parajuli 1191–1198

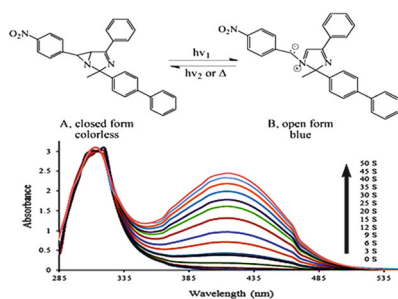
Computational study of ethanol complexes with H_2O , H_2S and HF molecules has been carried out using a MP_2 level of theory. Carbon bonding and hydrogen bonding interactions have been analyzed in this study for all the complexes.



Anti-oxidant activity of 6-gingerol as a hydroxyl radical scavenger by hydrogen atom transfer, radical addition and electron transfer mechanisms

Manish K Tiwari and P C Mishra 1199–1210

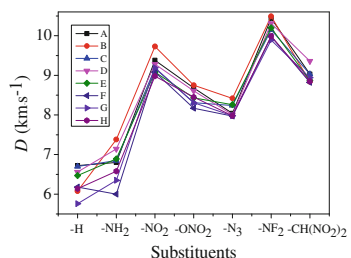
Hydrogen abstraction, radical adduct formation and single electron transfer as three mechanisms of antioxidant action of 6-gingerol as a hydroxyl radical scavenger have been investigated using transition state theory within the framework of density functional theory. 6-Gingerol is shown to be an excellent hydroxyl radical scavenger.



Synthesis, molecular structure, spectroscopic investigations and computational study of a potential molecular switch of 2-([1,1'-biphenyl]-4-yl)-2-methyl-6-(4-nitrophenyl)-4-phenyl-1,3-diazabicyclo [3.1.0]hex-3-ene

Ayoub Kanaani, Davood Ajloo, Hamzeh Kiyani, Freshte Shaheri and Majid Amiri 1211–1221

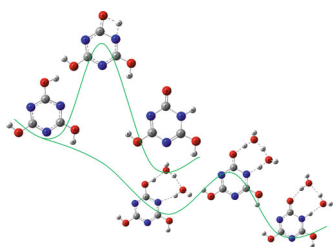
A novel photochromic compound was synthesized. The UV-Vis band in "A" form was observed at 310 nm (colorless), and for "B" form at 310 and 415 nm (blue color). The molecule is proposed as a potential photoinduced molecular switch for a molecular electronic device.



Design and selection of triazole-based compounds with high energetic properties and stabilities

Guozheng Zhao, Jianfeng Jia and Haishun Wu 1223–1236

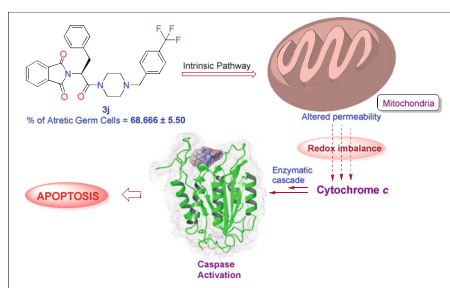
Density functional theory was used to study the energetic properties and thermal stabilities of the triazole derivatives. Twenty compounds may be considered as potential candidates with enhanced performance and reduced sensitivity. Thirteen compounds have better detonation properties than those of HMX (1,3,5,7-tetranitro-1,3,5,7-tetrazocane).



Effect of Mono- and Di-hydration on the Intramolecular Proton Transfers and Stability of Cyanuric Acid Isomers: A DFT Study

Younes Valadbeigi 1237–1244

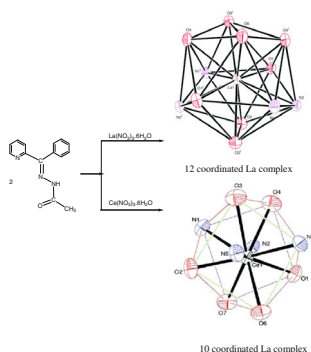
Cyanuric acid (CA) is a triazine molecule which exists in both keto and enol forms. The activation energies of the keto↔enol tautomerisms in CA are in the range of 130–210 kJ/mol. When the tautomerisms occur in the micro-hydrated isomers of CA, the water molecules catalyze the tautomerism and decrease the activation energies.



Design, synthesis and biological evaluation of Arylpiperazine-based novel Phthalimides: Active inducers of testicular germ cell apoptosis

Anil K Singh, Jitender K Bhardwaj, Ana Olival, Yogesh Kumar, Avijit Podder, Ankur Maheshwari, Renuka Agrawal, N Latha, Brajendra K Singh, Helena Tomás, João Rodrigues, Ram Kishan, B Rupini and Brijesh Rathi 1245–1263

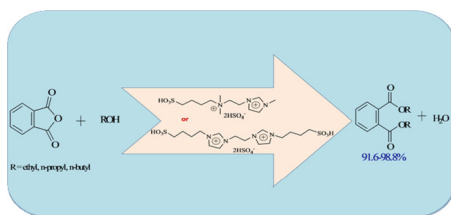
A new class of phthalimides functionalized with piperazines were prepared, characterized and validated as active inducers of apoptosis against testicular germ cells as advocated by histological and molecular techniques.



Synthesis, X-ray crystal structure, DNA binding and Nuclease activity of lanthanide(III) complexes of 2-benzoylpyridine acetylhydrazone

Karreddula Raja, Akkili Suseelamma and Katreddi Hussain Reddy 1265–1275

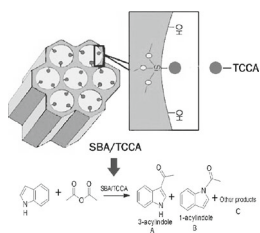
Lanthanide(III) complexes of general formula $[La(BPAH)_2(NO_3)_3]$ and $[Ce(BPAH)_2(NO_3)(H_2O)_2] \cdot 2NO_3 \cdot H_2O$ (where, BPAH = 2-benzoylpyridine acetyl hydrazone), were synthesized and characterized by elemental analysis, molar conductance, IR spectroscopy, single crystal X-ray diffraction and Hirshfeld studies. DNA binding and nuclease activity of these complexes were also investigated in the present work.



Functionalized dicationic ionic liquids: Green and efficient alternatives for catalysts in phthalate plasticizers preparation

Negar Zekri, Reza Fareghi-Alamdari and Zahra Khodarahmi. . . 1277–1284

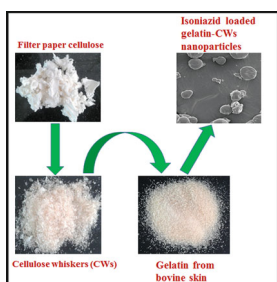
The synthesis route and characterization of two novel highly acidic ionic liquids, and the green and efficient synthesis of phthalate plasticizers in the presence of these ionic liquids are reported.



Synthesis and characterization of Trichloroisocyanuric acid functionalized mesoporous silica nanocomposite (SBA/TCCA) for the Acylation of Indole

G Robin Wilson and Amit Dubey 1285–1290

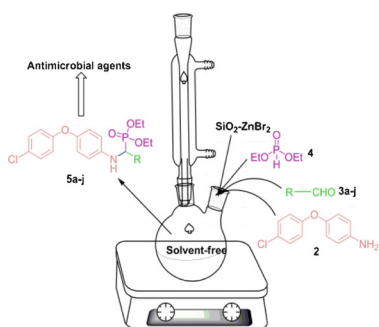
Synthesis of SBA-15/TCCA nanocomposites by *in situ* functionalization of ordered SBA-15 and acylation of indole in the liquid phase for higher selectivity of 3-acylated product are reported.



Isoniazid loaded gelatin-cellulose whiskers nanoparticles for controlled drug delivery applications

Mandip Sarmah, Anwar Hussain, Anand Ramteke and Tarun K Maji. 1291–1301

Isoniazid loaded gelatin-Cellulose Whisker nanoparticles were prepared by desolvation method and were characterized by X-ray diffractometry, Fourier Transform Infrared Spectroscopy, Scanning Electron Microscopy and Transmission Electron Microscopy. The nanoparticles have potential applications in the field of controlled drug delivery.



A heterogeneous catalyst, SiO₂-ZnBr₂: An efficient neat access for α-aminophosphonates and antimicrobial activity evaluation

Munichandra Reddy Sivala, Subba Rao Devineni, Madhava Golla, Venkatesh Medarametla, Gnana Kumari Pothuru and Naga Raju Chamarthi 1303–1313

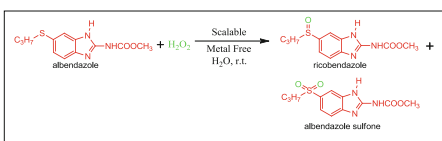
An efficient, neat and green method was developed for α-aminophosphonates by Kabachnik-Fields reaction using the catalyst, SiO₂-ZnBr₂. The developed method under conventional conditions was further optimized in microwave and ultrasonication methods. SiO₂-ZnBr₂ catalyst afforded good yields of the products (85–97%). Molecules were evaluated for antimicrobial activity including their MIC.



Curcuminoid-derived 3,5-bis(styryl)isoxazoles - Mechanochemical synthesis and antioxidant activity

Daisy R Sherin and Kallikat N Rajasekharan 1315–1319

Mechanochemical synthesis of curcuminoid-derived 3,5-bis(styryl)isoxazoles (4a-g) and their antioxidant activities are reported.

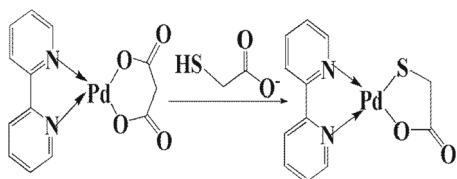


An eco-friendly oxidation of sulfide compounds

Ravindra B Wagh, Sitaram H Gund and Jayashree M Nagarkar 1321–1325

Using H₂O₂ as an oxidant and H₂O as the solvent, albendazole is oxidized to ricobendazole and albendazole sulfone.

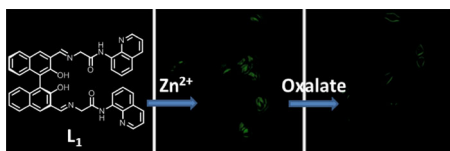
Substitution reactions of [Pd(bipy)(malonate)] explored with a different set of ligands: Kinetic and mechanistic interpretation in aqueous medium and at pH 7.4



Sumon Ray, Parnajyoti Karmakar, Animesh Chattopadhyay, Debabrata Nandi, Sushobhan Ukil, Roshni Sarkar (Sain) and Alak K Ghosh 1327–1335

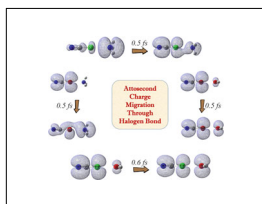
Studies of kinetic and mechanistic pathways for the reactions of Pd(II)-bipy-malonate complex with thioglycolic acid, thiourea and thiosemicarbazide have been carried out. Innermetallic [Pd(bipy)(malonate)] complex reacts with above mentioned sulphur containing ligands at physiological condition and these substitution reactions are associative in nature.

A fluorescent sensor based on binaphthol-quinoline Schiff base for relay recognition of Zn²⁺ and oxalate in aqueous media



Lijun Tang, Di Wu, Zhenlong Huang and Yanjiang Bian . . . 1337–1343

A new binaphthol-quinoline Schiff base-based fluorescent sensor **L₁** exhibits highly selective relay recognition of Zn²⁺ and oxalate through fluorescence “off-on-off” functionality in DMSO-H₂O (1/1, v/v, HEPES 10 mM, pH = 7.4) solution.



Cover picture: Electron-Electron Relaxation- and Correlation-Driven Charge Migration. For details, see the paper by S Chandra *et al.* (pp. 1175–1189)