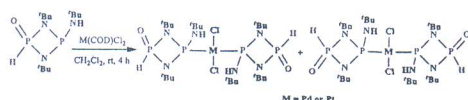


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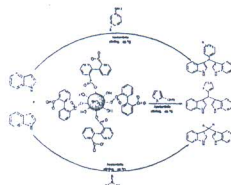
#### A mixed-valent cyclodiphosphazane: Transition metal chemistry and *cis/trans* isomerisation



Guddekoppa S Ananthnag, Joel T Mague and Maravanji S Balakrishna . . . . . 979–986

Transition metal complexes of a mixed-valent cyclodiphosphazane are described.

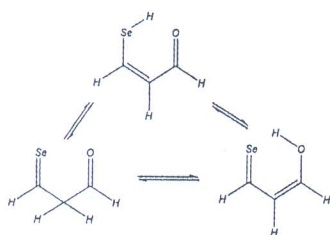
#### SiO<sub>2</sub>-Diphenic acid: An efficient and recyclable heterogeneous catalyst for one-pot synthesis of *bis*-(indolyl)methane derivatives in liquid phase



R Vaid, M Gupta, O S Chambyal and R Gupta . . . . . 987–997

The aim of this work is to highlight the efficiency and suitability of silica-diphenic acid as a supported solid acid catalyst for the synthesis of *bis*-(indolyl)methane derivatives from a one-pot condensation reaction of various substituted aldehydes and indole in acetonitrile at 60°C.

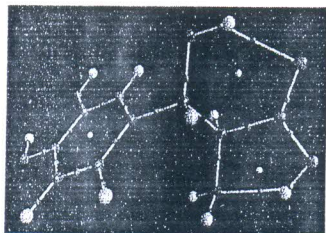
#### A comprehensive study of the structure, tautomeric properties, and conformational flexibility of 3-Hydroxy-propeneselenal



Mehdi Yoosefian, Heidar Raissi and Saeedeh Soheili . . . . . 999–1006

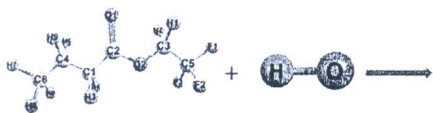
3-Hydroxy-propeneselenal has 20 different possible conformers as can be observed from an analysis of the structure. On the basis of functional groups, these conformers can be grouped into three tautomeric classes: HP, SP and SOP, which have 8, 8 and 4 rotamers, respectively.

#### A theoretical study of solvent effects on the characteristics of the intramolecular hydrogen bond in Droxidopa



Mehdi Yoosefian, Hassan Karimi-Maleh and Afsaneh L Sanati . . . . . 1007–1013

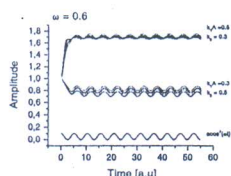
The molecular structures of Droxidopa have been investigated with density functional theory. A computational study of a representative number of actual and model structures was carried out in five solvents with different polarities: water, ethanol, carbon tetrachloride, dimethyl sulfoxide, and tetrahydrofuran, utilizing the polarizable continuum model.



**Theoretical study on mechanism, kinetics, and thermochemistry of the gas phase reaction of 2,2,2-trifluoroethyl butyrate with OH radicals at 298 K**

Nand Kishor Gour, Bhupesh Kumar Mishra and  
Hari Ji Singh . . . . . 1015–1023

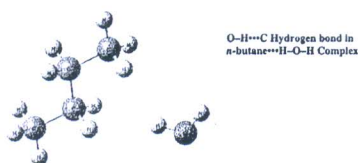
The reaction kinetics of H-atom abstraction reaction of 2,2,2-trifluoroethyl butyrate (TFEB) with OH radicals was investigated at M06-2X/6-31+G (d,p) level of theory. The branching ratios of the different reaction channels are also determined. The atmospheric lifetime of TFEB is estimated to be 6.8 days.



**Mathematical description of the nonlinear chemical reactions with oscillatory inflow to the reaction field**

Aldona Krupka . . . . . 1025–1034

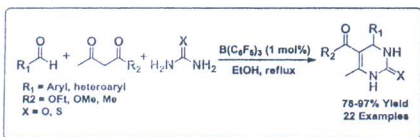
Approximate analytical solution is proposed for the nonlinear autocatalytic chemical processes with a time-varying and oscillating inflow of reactant to the reaction medium.



**X-H...C hydrogen bonds in *n*-alkane-HX (X = F, OH) complexes are stronger than C-H...X hydrogen bonds**

R Parajuli and E Arunan . . . . . 1035–1045

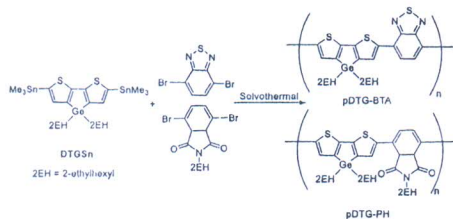
O-H...C hydrogen bond in *n*-butane represents *n*-alkane-HX (X = F, OH) complexes. X-H...C hydrogen bonds are found to be stronger than C-H...X hydrogen bonds.



**B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> catalyzed one-pot three-component Biginelli reaction: An efficient and environmentally benign protocol for the synthesis of 3,4-dihydropyrimidin-2(1H)-ones/thiones**

Santosh Kumar Prajapati, Keshav Kumar Gupta and  
Bathini Nagendra Babu . . . . . 1047–1052

*Tris*(pentafluorophenyl)borane catalyzed, one-pot, simple, efficient and environmentally benign protocol for the synthesis of dihydropyrimidinones/thiones *via* Biginelli reaction has been described.



**Solvothermal synthesis of high molecular weight dithienogermole containing conjugated polymers**

Fei-Bao Zhang, Su-Fang Lv, Jiang-Xiong Jiang and  
Yong Ni . . . . . 1053–1056

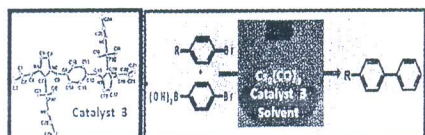
Synthesis and characterization of a new dithienogermole-diphthalimide and dithienogermole-dithiadiazole alternate polymers *via* the solvothermal method are reported.



***N,N'*-Olefin functionalized *Bis*-Imidazolium Pd(II) chloride *N*-Heterocyclic carbene complex builds a supramolecular framework and shows catalytic efficacy for 'C-C' coupling reactions**

Gourisankar Roymahapatra, Tapastaru Samanta, Saikat Kumar Seth, Ambikesh Mahapatra, Shyamal Kumar Chattopadhyay and Joydev Dinda. . . . . 1057–1065

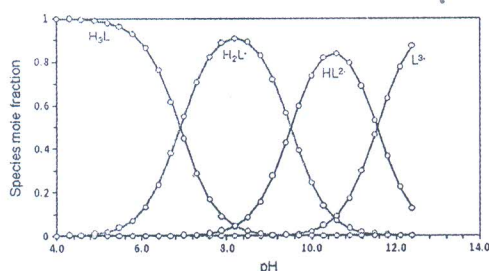
Palladium(II) *N*-heterocyclic carbene (NHC) complex (**3**) of the ligand 3,3'-(*p*-phenylenedimethylene)bis{1-(2-methylallyl)}imidazolium bromide has been synthesized and characterized by several spectroscopic techniques and finally the solid-state structure of **3** has been determined by single-crystal X-ray diffraction studies. The Pd(II) complex possesses ring head to tail  $\pi$ - $\pi$  stacking interaction (3.767 Å) through imidazole rings. Complex **3** catalyzes Suzuki–Miyaura 'C-C' coupling reaction. DFT calculations were performed to know HOMO/LUMO energy and hence the stability and reactivity of Pd(II) complex in *syn*- and *anti*-configuration.



**Thermodynamic modeling of naringenin protonation equilibria in NaClO<sub>4</sub> aqueous solutions by specific ion interaction theory and Pitzer equations**

Morteza Jabbari, Rahele Zhiani and Ali Farajtabar . . . . . 1067–1074

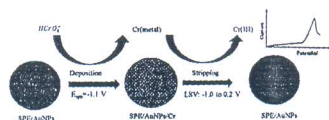
Ionic strength dependence of protonation constants for the flavonoid naringenin was investigated at 25°C using combined spectroscopic and potentiometric methods in different aqueous solutions of NaClO<sub>4</sub> (0.10–3.00 mol dm<sup>-3</sup>). The SIT and Pitzer equations were used for thermodynamic modeling of dependence on ionic strength of the protonation equilibria.



**Linear sweep anodic stripping voltammetry: Determination of Chromium (VI) using synthesized gold nanoparticles modified screen-printed electrode**

Salamatu Aliyu Tukur, Nor Azah Yusof and Reza Hajian . . 1075–1081

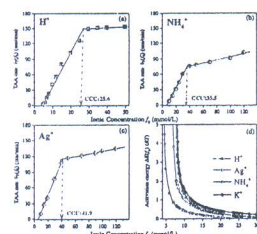
An electrochemical sensor has been constructed based on screen-printed electrode (SPE) modified with gold nanoparticles for determination of Cr(VI) ion in water samples. The coupling of anodic stripping voltammetry with SPE-modified nanostructures enhanced the sensitivity of electrochemical sensor for detection of Cr(VI) ion at low sample volumes.



**Observation of the Unusual Aggregation Kinetics of Colloidal Minerals in Acidic Solutions**

Rui Tian, Gang Yang, Xinmin Liu, Chengzhi Huang, Xiaodan Gao and Hang Li . . . . . 1083–1089

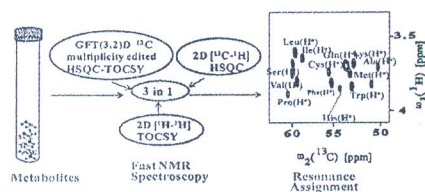
The aggregation kinetics of montmorillonite colloids in H<sup>+</sup>, Ag<sup>+</sup>, NH<sub>4</sub><sup>+</sup>, K<sup>+</sup> and Na<sup>+</sup> solutions were measured *in situ*, detecting the unusual kinetics and ion specificity for H<sup>+</sup>. It has been substantiated that the unusual ion specificity of H<sup>+</sup> is caused by steric effect.



**Simultaneous acquisition of three NMR spectra in a single experiment for rapid resonance assignments in metabolomics**

Shivanand M Pudakalakatti, Abhinav Dubey and Hanudatta S Atreya . . . . . 1091–1097

We describe here a first application of a combination of different fast NMR methods to simultaneously acquire three spectra in a single data set. The method combines G-matrix Fourier transform (GFT) NMR spectroscopy, parallel data acquisition and non-uniform sampling. This opens up new avenues for high-throughput approaches in metabolomics.







### Computational studies on 1,2,4-Triazolium-based salts as energetic materials

Rakhi Singh, Hari Ji Singh and S K Sengupta . . . . . 1099–1107

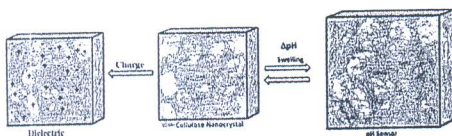
Condensed phase heats of formation of the designed triazolium-based ionic salts and their thermodynamic and energetic properties have been determined using computational methods. The calculated energetic properties indicate that the  $-\text{NO}_2$  and the  $-\text{N}_3$  groups are the effective explosophores for enhancing the detonation performance of the substituted triazolium cations.



### Effect of external electric field on Cyclodextrin-Alcohol adducts: A DFT study

Kundan Baruah and Pradip Kr Bhattacharyya . . . . . 1109–1117

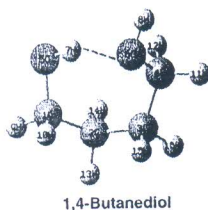
Cyclodextrin-alcohol adducts show remarkable response towards the strength and direction of the applied electric field.



### Designing pH-responsive and dielectric hydrogels from cellulose nanocrystals

Xiaoyuan Gao, Kishor Kumar Sadasivuni, Hyun-Chan Kim, Seung-Ki Min and Jaehwan Kim . . . . . 1119–1125

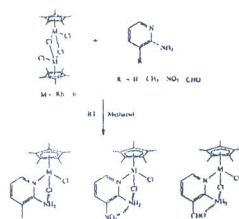
A pH-responsive hydrogel with improved mechanical and dielectric properties prepared from cellulose nanocrystals is reported. The resulting pH hydrogel exhibits a pronounced change in their swelling index in response to variation in pH. It also illustrates significant improvement in the dielectric constant which is thus useful in energy storage applications.



### Intramolecular hydrogen bond: Can it be part of the basis set of valence internal coordinates in normal mode analysis?

Sarvesh Kumar Pandey, Prasanta Das, Puspendu K Das, Elangannan Arunan and Sadasivam Manogaran . . . . . 1127–1134

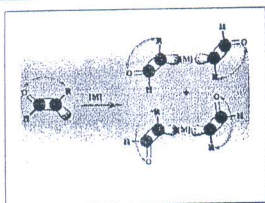
The relaxed force constants (RFCs) could be used as a measure of bond strength when the bonds are part of the basis. We define more than one 'equivalent' complete VIC basis sets where the intramolecular hydrogen bond is part of at least one of the basis sets.



### Half-sandwich pentamethylcyclopentadienyl group 9 metal complexes of 2-aminopyridyl ligands: Synthesis, spectral and molecular study

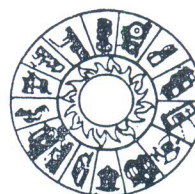
Mahesh Kalidasan, Scott Forbes, Yuriy Mozharivskyj and Mohan Rao Kollipara . . . . . 1135–1144

A new series of pentamethylcyclopentadienyl rhodium/ iridium complexes with 2-aminopyridyl ligands have been synthesized and characterized by spectral studies. The complexes have shown that piano-stool geometry around the metal center in which 2-aminopyridyl ligand acts as an N-mono-dentate ligand and the amino functionality is never involved in metal coordination.



Cover picture: *cis-trans* isomerization of cyclodiphosphazane. For details, see the paper by Guddekoppa S Ananthnag *et al.* (pp. 979–986)





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