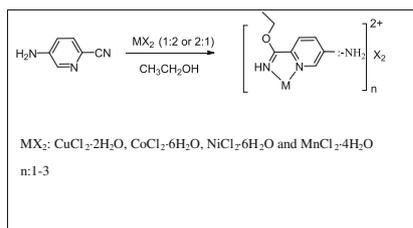


CONTENTS

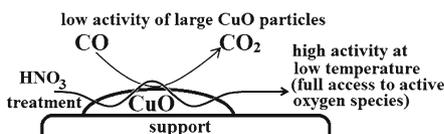
Rapid Communications



Synthesis and catalytic activity of metallo-organic complexes bearing 5-amino 2-ethylpyridine -2-carboximidate

Luo Mei, Xu Jia and Zhang Jing Cheng 855–860

Reaction of 5-amino-2-cyanopyridine with $\text{MCl}_2 \cdot x\text{H}_2\text{O}$ (M : Cu^{2+} , Co^{2+} , Ni^{2+} , Mn^{2+}) in anhydrous ethanol resulted in the production of four complexes. Their structures were determined by X-ray diffraction, NMR, IR, and elemental analysis. These complexes were then used as a catalyst in the Henry reaction.

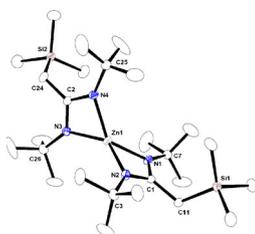


Catalytic activity of $\text{CuO-Gd}_{0.1}\text{Ti}_{0.1}\text{Zr}_{0.1}\text{Ce}_{0.7}\text{O}_2$ in CO oxidation

Igor V Zagaynov and Elena Yu Liberman 861–865

(1-10 wt.%) $\text{CuO-Gd}_{0.1}\text{Ti}_{0.1}\text{Zr}_{0.1}\text{Ce}_{0.7}\text{O}_2$ mesoporous catalysts show the highest activity of CO oxidation (full conversion at temperature of 60-65°C) due to better dispersion of CuO particles and enhanced interaction between CuO and the developed support based on ceria solid solution.

Regular Articles



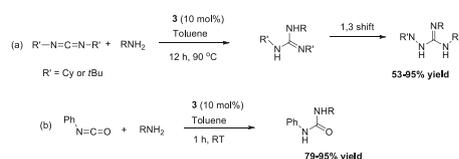
Amidinate Ligands in Zinc coordination sphere: Synthesis and structural diversity

Srinivas Anga, Indrani Banerjee and Tarun K Panda. 867–873

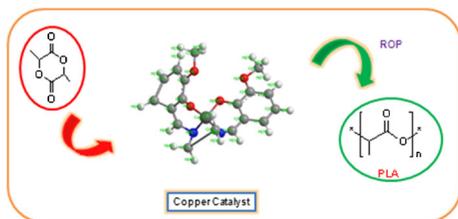
We report the syntheses and structural characterization of three homoleptic zinc amidinate complexes derived from one-pot reaction of carbodiimides ($\text{RN}=\text{C}=\text{NR}$, R = cyclohexyl, isopropyl, tert-butyl), neosilyllithium and anhydrous zinc chloride in diethyl ether at ambient temperature 25 °C.

Zinc catalyzed Guanylation reaction of Amines with Carbodiimides/Isocyanate leading to Guanidines/Urea derivatives formation

Jayeeta Bhattacharjee, Mitali Sachdeva, Indrani Banerjee and Tarun K Panda. 875–881



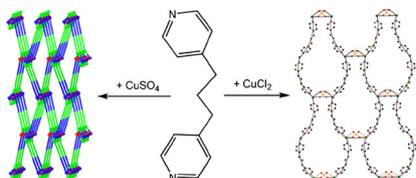
We report the highly chemo-selective catalytic addition of N–H bonds from various aromatic amines to carbodiimides and isocyanates using (Ar-BIAO)ZnCl₂ complex [Ar-BIAO = *N*-(2,6-diisopropylphenyl)imino-acenaphthenone, (**3**)] as the pre-catalyst to prepare guanidine and urea derivatives in 53-90% and 79-95% yield, respectively.



Salicylaldimine Copper(II) complex catalyst: Pioneer for ring opening Polymerization of Lactide

Anita Routaray, Nibedita Nath, Tungabidya Maharana,
Pratap Kumar Sahoo, Jaya Prakash Das
and Alekha Kumar Sutar 883–891

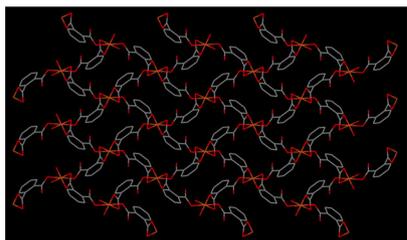
This article describes the synthesis and characterization of salicylaldimine copper(II) complexes, and their catalytic activity towards ring-opening polymerization of L-lactide.



Synthesis and structures of two new Cu(I) frameworks bearing 1,3-bis(4-pyridyl)propane and inorganic linkers

Zhaobo Hu, Bo Li, Wenqiang Ju, Yuning Liang
and Zilu Chen 893–898

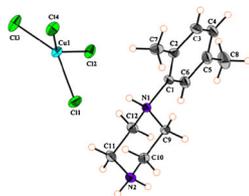
We present two typical metal-organic frameworks of Cu(I) constructed by the synergistic use of organic and inorganic linkers, which feature 3,3,4-connected 3-nodal 3D network and 2D framework with flask-stacking appearance.



Synthesis, crystal structure and Thermogravimetry of ortho-phthalic acid bridged coordination polymer of Copper(II)

Babita Sarma, Saurav Bharali and Diganta Kumar Das 899–904

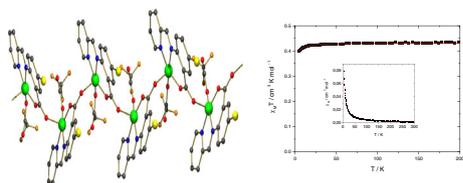
The reaction of $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ with (2-butoxycarbonyl)benzoic acid yielded three dimensional coordination polymer where *o*-phthalic acid acts as bridge between Cu(II) centres. The X-ray crystal structure shows monoclinic $P2_1/c$ space group with one carboxylate of *o*-phthalic acid binding to one Cu(II) as bidentate while the other carboxylate binding to another Cu(II) as monodentate.



Synthesis, crystal structure and magnetic properties of 1-(2,5-dimethylphenyl) piperazine-1,4-dium tetrachloridocuprate(II)

L Khedhiri, Jin-Xiao Mi, M Rzaigui and C Ben Nasr 905–911

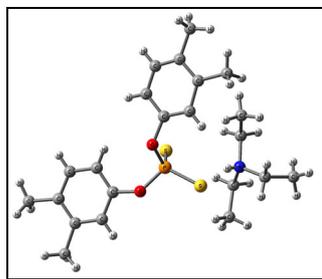
The synthesis and physico-chemical characterization of a novel organic-inorganic hybrid material, 1-(2,5-dimethylphenyl)piperazine-1,4-dium tetrachloridocuprate(II), are reported.



Crystal structure, characterization and magnetic properties of a 1D copper(II) polymer incorporating a Schiff base with carboxylate side arm

Shyamapada Shit, Madhusudan Nandy, Corrado Rizzoli,
Cédric Desplanches and Samiran Mitra 913–920

Syn-anti $\mu_{1,3}$ - bridging mode of the side arm carboxylate oxygen atoms of the coordinated Schiff base result in a zigzag 1D copper(II) chain complex, $[\{\text{Cu}(\text{L})(\text{CF}_3\text{COO})\}_2]_n$, which shows antiferromagnetic interaction ($J = -0.47 \pm 0.01 \text{ cm}^{-1}$).



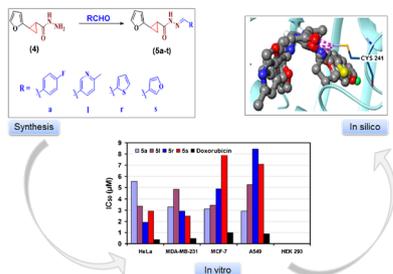
Triethylammonium salt of dimethyl diphenyldithiophosphates: Single crystal X-ray and DFT analysis

Sandeep Kumar, Ruchi Khajuria, Mandeep Kour, Rakesh Kumar,
Love Karan Rana, Geeta Hundal, Vivek K Gupta, Rajni Kant
and Sushil K Pandey 921–928

DFT studies of the structural (geometries, bond lengths and bond angles) and spectroscopic properties (vibrational and HOMO–LUMO) of aromatic dithiophosphates are reported and compared with experimental results for the first time.

Synthesis, biological evaluation and molecular docking studies of some novel cyclopropane carbohydrazone derivatives as potential anticancer agents

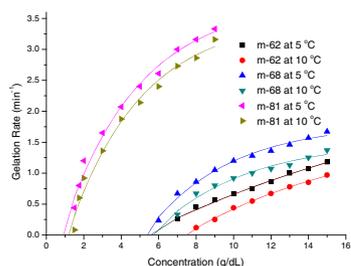
Ponnappalli Veerabhadra Swamy, Pullaiah China Kambhampati, Kothapalli Bonnoth Chandrasekhar, Gugulothu Thirupathi, Pombala Sujitha, Chityal Ganesh Kumar and Veeramachaneni Ganesh Kumar . . . 929–939



Synthesis of substituted N-hetero/arylidene-2-(furan-2-yl) cyclopropane carbohydrazides is reported. These compounds were screened for anticancer activity against four cancer cell lines. Four compounds showed promising activity at micromolar concentration against with IC₅₀ values ranging between 1.9-8.45 µM.

Effect of Isotacticity of Linear Poly(N-isopropylacrylamide) on its Gelation in Benzyl Alcohol

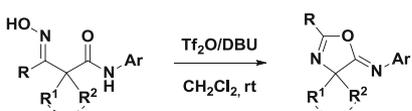
Chandra Sekhar Biswas, Kheyath Mitra, Shikha Singh, Dinesh K Patel, Biswajit Maiti, Pralay Maiti and Biswajit Ray 941–950



Thermoreversible gelation of different isotactic [meso diad (*m*) = 62, 68 and 81%] linear poly(*N*-isopropylacrylamide) (PNIPAM)s has been observed in benzyl alcohol. Gelation rate depends on temperature, concentration, and isotacticity of PNIPAM. SEM, XRD, rheology and UV-Vis studies, and molecular modelling support its formation presumably *via* polymer-solvent compound formation.

Triflic Anhydride-Mediated Beckmann Rearrangement Reaction of β-Oximyl Amides: Access to 5-Imino oxazolines

Mangfei Yu, Qian Zhang, Jia Wang, Peng Huang, Pengfei Yan, Rui Zhang and Dewen Dong 951–956

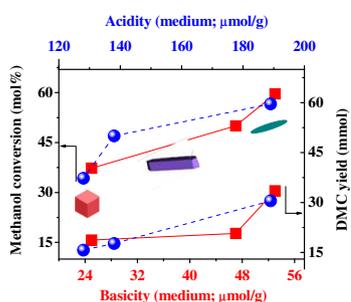


- One C-C Bond Cleavage
- One C-N Bond Formed
- One Ring Formed
- One O-C Bond Formed

Facile and efficient synthesis of 5-imino oxazolines from α,α-disubstituted β-oximyl amides *via* tandem triflic anhydride-mediated Beckmann rearrangement and intramolecular cyclization reaction under very mild conditions is described.

Direct synthesis of dimethyl carbonate from CO₂ and methanol over CeO₂ catalysts of different morphologies

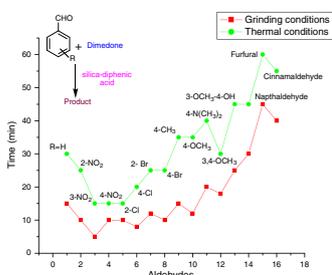
Unnikrishnan P and Srinivas Darbha 957–965



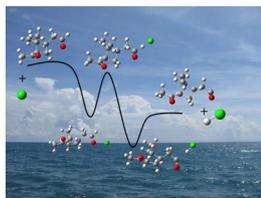
Direct synthesis of dimethyl carbonate from CO₂ and methanol in presence of 2-cyanopyridine as water trapping agent was studied with CeO₂ of different morphologies as a catalyst. Catalytic activity correlates with the amount of acid/base sites of medium strength, defect sites and exposed (111) facets. CeO₂ with spindle morphology shows superior catalytic performance compared to rod, cube and irregular or ‘no-definite’ shape morphologies.

Domino Knoevenagel/Michael synthesis of 2,2'-arylmethylenebis(3-hydroxy-5,5-dimethyl-2-cyclohexen-1-one) derivatives catalyzed by silica-diphenic acid and their single crystal X-ray analysis

Rupali Vaid, Monika Gupta, Rajni Kant and Vivek K Gupta 967–976



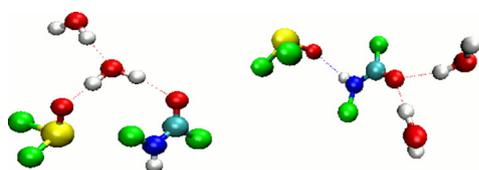
Silica-diphenic acid-catalyzed, efficient synthesis of 2,2'-arylmethylenebis(3-hydroxy-5,5-dimethyl-2-cyclohexen-1-one) derivatives is reported by reaction of different aldehydes with dimedone under grinding as well as thermal conditions. The structure-activity relationships and characterization of the different aldehydes used in the synthesis of these compounds have also been carried out.



Rate coefficients for hydrogen abstraction reaction of pinonaldehyde ($C_{10}H_{16}O_2$) with Cl atoms between 200 and 400 K: A DFT study

G Srinivasulu and B Rajakumar 977–989

The kinetics of the reaction between pinonaldehyde ($C_{10}H_{16}O_2$) and Cl atom were studied computationally and the rate coefficients computed in the temperature range between 200 and 400 K. The H abstraction reaction from the $-CHO$ group was found to be the most dominant reaction channel among all the possible reaction pathways.

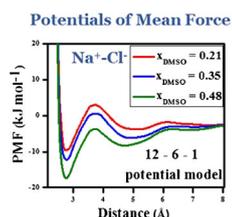


H-bonded species in aqueous NMA-DMSO solution.

Effects of dimethyl sulfoxide on the hydrogen bonding structure and dynamics of aqueous N-methylacetamide solution

Apramita Chand and Snehasis Chowdhuri 991–1001

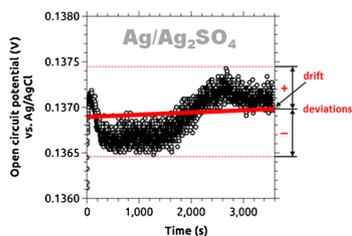
Classical molecular dynamics simulations have been carried out to investigate the influence of DMSO on the structure and dynamics of hydrogen bonds in aqueous NMA solutions. Properties like inter-species average interaction energies, self-diffusion coefficients, orientational relaxation times as well as hydrogen bond structural relaxation times and lifetimes have been calculated.



$Na^+ Cl^-$ ion pair association in water-DMSO mixtures: Effect of ion pair model potentials

Atanu Sarkar, Anupam Chatterjee, S C Tiwari
and B L Tembe 1003–1010

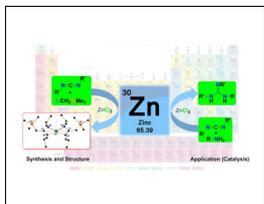
The effect of the differences between the 12-6-1, Huggins-Mayer (exp-6-1) and Fumi-Tosi (exp-6-8-1) ion-ion potential models on the solvation structure of the sodium chloride ion pair in water-DMSO binary mixtures have been studied.



Characterization of Ag/Ag_2SO_4 system as reference electrode for *in-situ* electrochemical studies of advanced aqueous supercapacitors

Denys G Gromadskyi 1011–1017

Silver sulfate reference electrode was developed to use as an alternative to the silver chloride for application in studies of the supercapacitor electrode materials. Ag/Ag_2SO_4 electrode demonstrates excellent potential stability during the two-hour electrochemical measurements in open-circuit mode.



Cover picture: Highly chemo-selective catalytic addition using zinc pre-catalysts. For details, see the paper by Jayeeta Bhattacharjee *et. al.* (pp. 875–881)