

Thermogravimetric Study of Ionic Pt(II) Complexes Containing *Bis*(diphenylthiophosphinyl)methane

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The TG-DTG and DTA study of dipositive platinum(II) complexes of the general formula $[\text{Pt}(\text{L-L})(\text{dppmS}_2)](\text{ClO}_4)_2$, where $\text{dppmS}_2 = \text{Ph}_2\text{P}(\text{S})\text{CH}_2\text{P}(\text{S})\text{Ph}_2$ and $\text{L-L} = \text{dppm}$ ($\text{Ph}_2\text{PCH}_2\text{PPh}_2$), dppe ($\text{Ph}_2\text{PCH}_2\text{CH}_2\text{PPh}_2$), and dppp ($\text{Ph}_2\text{PCH}_2\text{CH}_2\text{CH}_2\text{PPh}_2$), were studied by thermogravimetric analysis from ambient temperature to 1000°C in nitrogen atmosphere. The decomposition occurred in one stage for $[\text{Pt}(\text{L-L})\text{dppmS}_2](\text{ClO}_4)_2$, $[\text{Pt}(\text{L-L})\text{dpppS}_2](\text{ClO}_4)_2$ and $[\text{Pt}(\text{L-L})\text{dppmS}_2](\text{ClO}_4)_2$ complexes. The values of activation energy, E , frequency factor, A , reaction order, n , entropy change, ΔS^\ddagger , enthalpy change, ΔH^\ddagger , and Gibbs free energy change, ΔG^\ddagger , of the thermal decomposition were calculated by means of Coats-Redfern method (CR), MacCallum-Tanner method (MC) and van Krevelen method (vK). The activation energy values obtained by CR, MC and vK methods were in good agreement with each other.

Key words: thermal behaviour, ionic Pt(II) complexes, activation energy

The Reciprocal $\text{CuInSe}_2+2\text{CdTe}\rightleftharpoons\text{CuInTe}_2+2\text{CdSe}$ System

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Investigation of the reciprocal system $\text{CuInSe}_2+2\text{CdTe}\rightleftharpoons\text{CuInTe}_2+2\text{CdSe}$ was performed using XRD and differential thermal analysis. The isothermal section at 870 K, the liquidus surface projection, several vertical sections and a spatial diagram were constructed. The existence of a large homogeneity region of the sphalerite modifications of the compounds was established.

Key words: semiconductors, liquid-solid, phase diagrams, thermal analysis, XRD analysis

The Elimination of Cadmium(II) from Aqueous Environment by Supported Liquid Membrane Method Using the Basic Carrier

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The transport of cadmium ions through a supported liquid membrane containing triethanolamine (TEA) as a mobile carrier has been studied. The effects of Cd(II) concentration, HCl in feed and carrier concentration in membrane have been studied. Cd(II) concentration increase in feed leads to an increase in flux from 2.1×10^{-7} to 8.4×10^{-7} mol cm⁻² sec⁻¹ within Cd(II) ions concentration range (2.7×10^{-4} M – 16.3×10^{-4} M) at 2.0 M HCl in the feed and 3.0 M triethanolamine in the membrane. Increase in H⁺ ion concentration from 0.5 M to 3.0 M results in an increase in Cd(II) ions flux but a decrease is observed beyond 2.0 M HCl concentration in feed. Increase in carrier concentration in the liquid inside the membrane enhances the flux with its maxima at 3.0 M carrier. Further increase in the concentration of TEA leads to a decrease in transport due to increase in viscosity of membrane liquid. The optimum conditions for Cd(II) ions transport are, 2.0 M HCl in feed, 3.0 M TEA in membrane and 0.1 M NaOH as strip solution. Similar transport characteristics have been observed for Cd-EDTA complexed anions across TEA-cyclohexanone based SLM, thus indicating a cadmium anion transport coupled with protons and chloride or EDTA co-ions.

Key words: cadmium, triethanolamine, supported liquid membrane, waste effluent

**Synthesis, Crystal Structures and
Antifungal Activities of Two Isostructural
Dinuclear Zinc(II) Complexes Derived from
4-Chloro-2-[(2-methylaminoethylimino)methyl]phenol**

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Two new isostructural zinc(II) complexes with the formula $Zn_2L_2X_2$ (L = 4-chloro-2-[(2-methylaminoethylimino)methyl]phenolate; X = Br for (1) and Cl for (2)), have been synthesized from the reaction of the Schiff base ligand HL with zinc(II) halides in methanol solutions. The complexes have been structurally characterized by IR spectra and single-crystal X-ray diffraction. In each of the complexes, one Zn atom is in a distorted octahedral coordination, while the other Zn atom is in a distorted tetrahedral coordination. The distances between the two zinc centers are 3.126(1) Å for (1) and 3.128(1) Å for (2). The Schiff base ligand HL and the two complexes showed moderate antifungal activity against the fungi *Aspergillus flavus*, *Fusarium* and *Candida albicans*.

Key words: Schiff base, zinc(II) complex, synthesis, crystal structure, antifungal activity

Bimetallic Ag(I)-Cu(II) Assembly with Extended Oxamido-Bridged: Synthesis, Crystal Structure and Magnetism

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A new bimetallic compound $\text{Cu}_2(\text{oxae})(\text{H}_2\text{O})_2\text{Ag}_2(\text{CN})_4$ (**1**) (oxae = N,N'-bis(2-aminoethyl)oxamido dianion) was isolated and structurally characterized. Compound **1** crystallizes in the monoclinic system, with space group $P2_1/c$ and unit cell constants $a = 14.033(18)$, $b = 7.165(9)$, $c = 9.378(12)$ Å, $\beta = 103.890(14)^\circ$ and $Z = 2$. The complex **1** consists of the oxamido-bridged binuclear copper(II) unit and two linear cyanoargentate anions acting as monochelate ligands. The coordinated environment of the Cu atom is a square prism. The complex **1** is self-assembled into three-dimensional (3D) network *via* hydrogen bonds. The magnetic properties of **1** have been studied as well.

Key words: cyanoargentate, crystal structure, magnetic property, hydrogen bond, argentophilic interaction

Influence of Gelation Temperature on the Properties of Sol-Gel-Derived Calcium Hydroxyapatite Ceramics

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An aqueous sol-gel chemistry synthesis route has been developed to prepare calcium hydroxyapatite ($\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$, CHA) samples at different gelation temperatures. In the sol-gel processes, an aqueous solution of tartaric acid as complexing agent was used. The phase transformations, composition and micro-structural properties of the polycrystalline samples were studied by thermogravimetric analysis (TG), differential thermal analysis (DTA), energy-dispersive spectrometry (EDS), Fourier transform infrared spectroscopy (FTIR), X-ray powder diffraction analysis (XRD) and scanning electron microscopy (SEM). It was clearly demonstrated that temperature of initial stage of the preparation of CHA is a crucial parameter to obtain monophasic calcium hydroxyapatite powders with desired morphological properties.

Key words: biomaterials, calcium hydroxyapatite, sol-gel preparation

A Convenient Synthesis of 1-(ω -Aminoalkyl)-5-nitro-1*H*-pyrimidine-2,4-diones

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Several monoacylated alkylene diamines have been obtained in the reaction of appropriate amine with methyl phenylacetate or ethyl formate. The mono protected diamines were used as alkylating agents in reactions with 1-(2,4-dinitrophenyl)-5-nitrouracil. The series of hitherto unknown 1-(ω -aminoalkyl)-5-nitrouracil derivatives have been obtained as a result of the uracil ring transformation. The best yield of 1-(ω -aminoalkyl)-5-nitrouracils was obtained when *N*-Boc protected alkylene diamines were applied in this reaction. The *N*-Boc protecting group was cleaved using diluted trifluoroacetic acid, and the liberated amines were subjected to reaction with phthalic anhydride and naphthalene 1,8-dicarboxylic anhydride.

Key words: 1,3-diaminopropane, 1,4-diaminobutane, 1,6-diaminohexane, 5-nitrouracil, phthalic anhydride, naphthalene 1,8-dicarboxylic anhydride, *ANRORC* type reaction

Syntheses of *N,S*-Substituted 4-Chloro-2-mercapto-5-methylbenzenesulfonamide Derivatives with Potential Biological Activity

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The syntheses of *N,S*-substituted 4-chloro-2-mercapto-5-methylbenzenesulfonamide derivatives are described. The compounds **6–11**, **14**, **15** and **19–22** were tested for their *in vitro* anticancer activity against 9 human cancer cell lines. The most active compounds **6**, **9** and **20** showed moderate cytotoxic activity and were approximately 5-fold less potent than cisplatin.

Key words: *N,S*-substituted benzenesulfonamide derivatives, syntheses, anticancer activity

Synthesis of New Type of Vitamin E Glycoconjugates

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New type of α -tocopheryl glycoconjugate containing 5-carbon linker was described. The α -tocopheryl allyl ether was combined to peracetylated 3-butenyl α -mannopyranoside by cross metathesis. Transformation of the linker to easier cleavable enol ether was attempted.

Key words: α -tocopherol, glycoconjugate, cross metathesis, isomerization to enol ether

Synthesis of Conjugates of Amino-Combretastatin with Tuftsin Derivatives as Potential Anticancer Agents

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Novel 3'-*N*-(tuftsin or retro-tuftsin)-amino-combretastatin conjugates have been synthesized as potential anticancer compounds. We hope that the conjugation of immunomodulators like tuftsin derivatives with amino-combretastatin A-4 would improve the therapeutical properties of combretastatin A-4.

Key words: combretastatin A-4, CA-4, amino-combretastatin, retro-tuftsin, tuftsin, synthesis

On Chemical Bonding Between Helium and Oxygen

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A brief analysis of the He–O chemical bond, present in cationic (HeO⁺⁺) and a few hypothetical anionic species (XHeO⁻, X = F, Cl), is performed at various levels of theory. We are also able to propose two candidates for the first metastable neutral molecule which contains helium chemically bound to oxygen: (HeO)(CsF) and (HeO)(NMe₄F).

Key words: helium, Density Functional Theory, noble gases, post Hartree-Fock methods

Photocatalytic Oxidation of Cyclohexene with Molecular Oxygen Using Immobilized Vitamin B₁₂ within Nanoreactors of Al-MCM-41

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Immobilized vitamin B₁₂ within nanoreactors of Al-MCM-41 (Vit.B₁₂/Al-MCM-41) was used as catalyst in the photooxidation of cyclohexene with molecular oxygen in CH₃CN using medium pressure mercury lamp at room temperature. It was found that 99% of cyclohexene was converted to 2-cyclohexene-1-one (70%), 2-cyclohexene-1-ol (15%) and cyclohexene oxide (15%). Details of reaction are discussed.

Key words: photooxidation, vitamin B₁₂, Al-MCM-41

Spectrokinetic Study of the Reaction System of $2\text{NO}_2 \leftrightarrow \text{N}_2\text{O}_4$ with Butanols Between 320–358 K in the Gas Phase

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Spectrokinetic studies of the gas-phase equilibrium between nitrogen tetroxide and butanols in the reaction system $2\text{NO}_2 \leftrightarrow \text{N}_2\text{O}_4$ (1, 2), $\text{N}_2\text{O}_4 + \text{ROH} \leftrightarrow \text{RONO} + \text{HNO}_3$ (3, 4) have been undertaken in the temperature range 298–358 K. The products – RONO (*n*-butyl-ONO, *sec*-butyl-ONO, *iso*-butyl-ONO and *tert*-butyl-ONO) – were identified by their UV spectra and the values of the maxima UV absorption cross sections were determined in the range 320–420 nm at 298 K. The temperature dependences of both the forward and reverse rate constants, k_3 and k_4 , were obtained. The extrapolated values of the forward rate constants are $10^{-18} \text{ k}_3^{\text{av}}/\text{cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ 3.9±1.0; 1.7±0.3; 4.2±0.8; 5.7±1.1 and the reverse rate constants are $10^{-20} \text{ k}_4^{\text{av}}/\text{cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ 0.3±0.1; 2.3±0.6; 0.4±0.1; 2.3±0.6 at 298 K for the reaction of $\text{NO}_2/\text{N}_2\text{O}_4$ with *n*-butanol, *sec*-butanol, *iso*-butanol and *tert*-butanol, respectively. The activation energy for the forward E_3 and for the reverse E_4 reaction were derived.

Key words: nitrogen dioxide, dinitrogen tetroxide, butanols

Density Functional Study of ^{27}Al and ^{14}N Quadrupole Coupling Constants in the Carbon Doped (4,4) Single-Walled Armchair Aluminum Nitride Nanotube

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Density functional theory (DFT) calculations are carried out to study the influence of carbon doping (C-doping) on the aluminum-27 and nitrogen-14 quadrupole coupling constants (C_Q) in a representative model of aluminum nitride nanotubes (AINNTs). The model includes two perfect and C-doped forms of the (4,4) single-walled armchair AINNT. To this aim, each of two forms of AINNT is firstly optimized and then the electric field gradient (EFG) tensors are calculated and converted to C_Q . Comparison of the calculated C_Q values in two perfect and C-doped forms of AINNT reveals that the influence of C-doping is significant at the sites of the nearest Al and N nuclei while those nuclei far from the C atoms do not show changes.

Key words: aluminum nitride, carbon doping, density functional theory, electric field gradient, nuclear quadrupole resonance

Investigations on the Electronic Transitions and Photofragmentation of Bromine Molecule

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The electronic transitions and excited-state fragmentation of bromine molecule have been studied within the visible-near UV continuum. The molar extinction coefficients in this study are derived by performing the wave packet simulations of nuclear motion. The quantum yields of the spin-orbit $\text{Br}^*(^2\text{P}_{1/2})$ product at the different photon frequencies are determined as well. Employing the time-dependent density functional theory (TDDFT), the five highest occupied and the five lowest unoccupied orbitals of Br_2 have been analyzed, the transition to $\text{C}^1\Pi_u$ state is found to be most probable in the visible-near UV absorption band.

Key words: electronic transitions, photofragmentation, absorption spectrum

Synthesis, Characterization and Catalytic Activity of Resin-based Diiron(III) Interphase Catalysts: Model for Methane Monooxygenase

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Three resin-based μ -oxo diiron(III) interface catalysts have been successfully prepared to model the functional properties of methane monooxygenase (MMO). The catalysts were characterized and exhibited the catalytic activities in the oxidation of alkanes to corresponding alcohols and ketones in acetonitrile at room temperature by 30% hydroperoxide (H_2O_2) or *tert*-butyl hydroperoxide (TBHP) as the oxidants. For 2,6-di-*tert*-butylphenol as the substrate, the C–C coupling was found in the two reaction systems. The reaction mechanisms were proposed with the predominant radical mechanism.

Key words: methane monooxygenase, interface catalyst, resin, catalytic activity

**Carbon Tetrachloride Decomposition
in Spark Discharge Plasma**

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