

Synthesis, Characterization and Anti-inflammatory Activity of Some Organotin(IV) Complexes

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The synthesis and characterization of new coordination compounds of some organotin(IV) chlorides with fexofenadine are reported; the ligand molecules appear to be bound to the tin atom through carbonyl oxygen atom. The structure of the synthesized compounds has been characterized by elemental analyses, and bonding in these complexes is discussed in terms of their IR, ¹H NMR and through Mössbauer studies. The spectroscopic results obtained are in full agreement with the proposed 1:1 stoichiometry. The synthesized complexes have been screened for anti-inflammatory effect. The results obtained showed that triphenyltin(IV) derivatives of fexofenadine exhibited promising anti-inflammatory effect as compared to the other tin(IV) derivatives of the same ligand.

Key words: fexofenadine, spectra, anti-inflammatory, organotin, coordination

Synthesis, Characterization and Antibacterial Activity of Triorganotin(IV) Complexes of 4-Methylphenol

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The triorganotin(IV) complex of composition $\text{Ph}_3\text{Sn}(\text{OArMe-4})$ has been synthesized in good yields by the reaction of Ph_3SnCl with $\text{Me}_3\text{SiOArMe-4}/\text{NaOArMe-4}$, while complexes of composition $\text{Me}_3\text{Sn}(\text{OArMe-4})$ and $n\text{-Bu}_3\text{Sn}(\text{OArMe-4})$ (where $-\text{OArMe-4} = -\text{OC}_6\text{H}_4\text{CH}_3\text{-4}$) have been obtained from the reaction of Me_3SnCl and $n\text{-Bu}_3\text{SnCl}$ with 4-methylphenol in the presence of triethylamine in carbon tetrachloride. The complexes have been characterized by elemental analyses, molar conductance measurements, molecular weight determination and IR, ^1H and ^{13}C NMR and mass spectral studies. Thermal behaviour of the complexes has been studied by TG and DTA techniques. The organotin(IV) complexes have also been screened for their antibacterial properties and are found to exhibit appreciable activity. The reactions of the complexes with 2-, 3-, 4-cyanopyridines yielded 1:1 adducts as confirmed by physicochemical and IR spectral data.

Key words: trialkyl and triaryltin chlorides, 4-methylphenol, spectral studies, antibacterial activity

The Influence of 2,2 -Bipyridine and 1-Amino-9,10-anthraquinone Side-Arm on Complexation Equilibria of Diaza-15-crown Ether in Various Solvents

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The influence of 2,2 -bipyridine and 1-amino-9,10-anthraquinone side-arm of diaza-15-crown ether on silver(I) complexation equilibria has been investigated in various non-aqueous solvents. The 2,2 -bipyridyl residue attached to the nitrogen atom of the macrocycle significantly controls the formation of 1:1 inclusion-type complexes by stabilizing silver ions inside the cavity. The addition of a second 2,2 -bipyridine or 1-amino-9,10-anthraquinone slightly changes the stability constants of diaza-15-crown ether complexes and as well 1:2 metal-to-ligand complexes. Ag_2L^{2+} , $\text{Ag}_2\text{L}_3^{2+}$ and $\text{Ag}_2\text{L}_3^{2+}$ have been found, depending on the type of ligand and solvent species of higher complexity. This has been proved by both spectrophotometric and potentiometric methods. Studies of substituted diaza-15-crown ethers were performed for comparison with an unsubstituted ligand.

Key words: azacrown ethers, bipyridine, equilibrium, silver(I)

Synthesis, Spectral Characteristics and Antitumor Activity of Tungstosilicic Polyoxometalate Containing 5-Fluorouracil

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A novel polyoxometalate compound with 5-fluorouracil $C_4H_4FN_2O_2H_3SiW_{12}O_{40} \cdot 12H_2O$ (FSW) was synthesized and its structure was analyzed using IR spectra, X-ray powder diffraction (XRD), ^{183}W NMR and TG. IR spectra and XRD indicate that FSW has a Keggin structure of heteropolyanion with a ring structure of 5-fluorouracil as expected. It was found by the analysis of the ^{183}W NMR spectra that the W atoms of FSW remain in the same chemical environment. The results of TG show that the compound has two weight-losing steps with certain degree of thermal stability. The present study uses 5-fluorouracil as the positive control group in the cytotoxicity tests of FSW on human renal embryonic cell HEK293 and the antitumor activity tests in cervical cancer cell Hela using the methyl thiazolyl tetrazolium method. The results obtained show that the therapeutic index of the new polyoxometalate compound is 0.75, higher than that of 5-fluorouracil.

Key words: polyoxometalate, compositional characteristics, cytotoxicity, antitumor activity

Immobilization of Catalase *via* Adsorption onto Natural and Modified Montmorillonit Analsim-Clay

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Immobilization of the enzyme catalase on natural and modified montmorillonit analsim-clays was investigated using a batch system. Such an immobilization does not result in enzyme inactivation and constitutes a valuable method for immobilizing catalase at high ionic strength. In the immobilization process, the effect of pH, ionic strength and reaction temperature were chosen as parameters. Furthermore the optimization of immobilization conditions were studied using data obtained from experimental results. For the free catalase and three different immobilized catalase enzymes, the optimum pH values 8, 7, 7 and 8; reaction temperature 30 °C; ionic strength 0.25 M were found. It was determined that enzyme activity for enzyme supported by natural clay was 73.3%, when it was retained during the storage at 4 °C for a period of 60 days. It was observed that storage and operational stabilities of the enzyme increased with immobilization. The results obtained show that montmorillonit analsim-clay is valuable and favourable support the simple adsorption of enzymes.

Key words: catalase, clay, immobilization, bovine liver

Synthesis and Characterization of O,O -Ditolyl-S-silylphosphorodithiolates

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Reactions of SiCl_4 or Me_3SiCl with sodium ditolylphosphorodithioates, (*o*-, *m*- or *p*- $\text{MeC}_6\text{H}_4\text{O}$) $_2\text{PS}_2\text{Na}$, in different molar ratios in chloroform under anhydrous conditions, resulted in the formation of the compounds [$\{(o-, m- \text{ or } p\text{-MeC}_6\text{H}_4\text{O})_2\text{PS}_2\}_n\text{SiCl}_{4-n}$] ($n = 1$ or 2) or [$(o-, m- \text{ or } p\text{-MeC}_6\text{H}_4\text{O})_2\text{PS}_2\text{SiMe}_3$] in 74–83% yield. These colorless, oily liquid compounds were characterized by elemental analysis, molecular weight determinations, IR and NMR (^1H , ^{13}C and ^{31}P) spectroscopic studies, which revealed an unidentate mode of bonding of the dithiophosphate moiety with silicon atom, leading to a P–S–Si linkage.

Key words: organosilicon; phosphorodithioate, dithiophosphate, organophosphorus and phosphorus-sulfur

New Ferrocenylpyridinium Salts with Bulk Second-Order Nonlinear Optical Properties

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Protonation of (*E*)-1-ferrocenyl-2-(pyridin-4-yl)-ethylene with (+)-camphor-10-sulfonic and picric acid afforded salts displaying high second harmonic generation (SHG) efficiencies (70 and 10 × urea, respectively). Powder X-ray diffraction study confirmed crystallization of these salts in a noncentrosymmetric space group (*P2*). The electronic structure of the cationic part of the salts was studied by the DFT method.

Key words: ferrocene, pyridinium, nonlinear optics, second harmonic generation, powder X-ray diffraction, DFT

Fungal Cells Permeabilization as a Convenient Tool of Bioreduction Enantioselectivity Control

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The application of nonionic detergents: Triton X100 and Tween 80, as permeabilizing agents was an effective tool allowing to control the asymmetric hydrogen transfer in the biocatalyzed, enantioselective reduction of acetophenone to the desired optical isomer of 1-phenylethanol. Depending on the permeabilization procedure, the application of *Geotrichum candidum*, after the Triton X100 was applied, resulted in the formation of the *R*-enantiomer (79% of chemical yield and 72% of e.e), whereas bioreduction following the use of Tween 80 led to the *S*-form of 1-phenylethanol (51% of yield and 93% of e.e).

Key words: yeasts, bioreduction, acetophenone, permeabilization

DFT Calculations of the Structure and Adsorption of HCO₃ Species on the Surface of Al₂O₃ Catalyst

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Density functional theory (DFT) calculations have been carried out to study the structure and adsorption of HCO₃ species on Al₂O₃ catalyst using MPW1PW91 function and the different basis sets of 6-31G, 6-311G, 6-311+G(d), DGDZVP, DGDZVP2, PVQZ, SDD, LANL2DZ, LANL2MB. The geometrical structures and vibration spectra were obtained with DFT methods and compared with the corresponding experimental values. Theoretical calculations show that the calculated IR spectra using MPW1PW91/6-311G, MPW1PW91/SDD and MPW1PW91/LANL2DZ methods are in good agreement with the experimental spectroscopic results.

Key words: DFT, vibration spectra, HCO₃ species

Au/Fe₃O₄ and Au/Fe₂O₃ Catalysts: Physicochemical Properties and Oxidation of CO and Propane

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Catalysts containing Au deposited on Fe₃O₄ (commercial Cerac) and on Fe₂O₃ were synthesized, characterized by XPS, XRD, Mössbauer spectroscopy, H₂TPR, isopropanol decomposition – a probe reaction of acid-base properties, and tested in oxidation of CO and C₃H₈. Au/Fe₃O₄ catalyst, containing a mixture of magnetite and maghemite (γ-Fe₂O₃) phases, was found to be more acidic containing more surface OH groups and less reducible than Au/α-Fe₂O₃ (hematite). The activity in oxidation of CO and propane was higher for Au/α-Fe₂O₃ catalyst as compared with Au/Fe₃O₄.

Key words: Au/FeO_x catalysts: physicochemical properties, oxidation of CO, oxidation of propane

Application of Molecular Descriptors to the Prediction of Retention in Organic Solvent Nanofiltration

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An attempt to apply the molecular descriptors for the characterization of retention of solutes in organic solvent nanofiltration has been performed. The descriptors were calculated using the program Dragon. The geometry of each solute molecule has been optimized using Gaussian[®]. Two linear equations relating the retention coefficient, R , with one or two descriptors have been tested using two sets of solutes. The first one ("soft" set) consisted of saturated and aromatic hydrocarbons (data of White, *J. Membr. Sci.*, **205**, 191 (2002)), the second one ("hard" set) contained the substituted aromatic hydrocarbons with heteroatoms (data of Geens *et al.*, *J. Membr. Sci.*, **281**, 139 (2006)). It has been found that the "soft" set of compounds is described reasonably well by both equations. The best descriptors belong to GETAWAY descriptors and Burden eigenvalues. Regarding the "hard" set of compounds only the 2-descriptors equation yields a satisfactory fitting of R . Here the 3D-MoRSE descriptors are the best for 7 of 14 membrane-solvent systems.

Key words: nanofiltration, organic solvent, retention, molecular descriptor

Reduction Study of Iron-Alumina Binary Oxide $\text{Fe}_{2-x}\text{Al}_x\text{O}_3$

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The comparative study of iron-aluminum binary oxides $\text{Fe}_{2-x}\text{Al}_x\text{O}_3$ (where $x = 2/3, 1, 4/3$) reduction behavior was investigated and the obtained bi-oxides were characterized by TPR, TG-DTA, BET and XRD methods. In hydrogen atmosphere three step reduction pathway for iron-aluminum binary oxide was found. Such reduction behavior appeared reasonably analogical to that characteristic of hematite type iron(III) oxide reduction $3\text{Fe}_2\text{O}_3 \rightarrow 2\text{Fe}_3\text{O}_4 \rightarrow 6\text{FeO} \rightarrow 6\text{Fe}$. The reduction for unimolar bi-oxide $\text{Fe}_{2-x}\text{Al}_x\text{O}_3$ ($x = 1$) can be expressed in following way: $4\text{FeAlO}_3 \rightarrow 2\text{Fe}_2\text{AlO}_4 \rightarrow 2\text{FeAl}_2\text{O}_4 + 2\text{Fe} \rightarrow 4\text{Fe}$ but the last step of reduction was not accomplished below 1000 °C. In air FeAlO_3 bi-oxide decomposes above 1300 °C, whereas exothermal dissociation $2\text{FeAlO}_3 \rightarrow \text{Al}_2\text{O}_3 + \text{Fe}_2\text{O}_3$ above 770 °C was confirmed in argon atmosphere.

Key words: iron oxide, iron-alumina binary oxide, binary oxide, TPR- H_2

**Asymmetric $p(\text{O})-\pi(\text{Triazine})$ Conjugation
in the Formally Symmetric
Bis(4,6-dimethoxy-1,3,5-triazinyl)
Ether in Its Crystal Structure**

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Reported is the crystal structure of a formally symmetric bis(*s*-triazinyl) ether obtained as a by-product in the acylation reaction of less reactive nucleophiles with 2-acyloxy-4,6-dimethoxy-1,3,5-triazines. The title ether shows conformational asymmetry evidenced by different orientations of the four methoxy groups and the two aromatic rings in relation to the central etheric plane. Differentiation of the two O–C(*triazine*) bond lengths of the bis(triazinyl) ether can be correlated with the angles between *s*-triazine rings with the central etheric plane, indicating different degree of conjugation of the two π -systems with a lone pair of the central oxygen atom. It seems that primary reason for the observed asymmetry is crystal packing, causing different orientations of methoxy groups, which in turn induced bond lengths alternation in the *s*-triazine rings affecting their conjugations with central O atom through AGIBA effect. The experimental observations are in agreement with *ab initio* calculation.

Key words: bis(*s*-triazinyl) ether, asymmetric conjugation, crystallographic asymmetry of symmetric ethers, AGIBA effect

Fragment-topological Descriptors for QSPR Estimation of the Normal Boiling Point Temperature of Normal and Branched Hydrocarbons

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The new QSPR correlation equation was developed for the estimation of the boiling points of special families of alkanes. This equation includes contributions depending on the total number of carbon atoms forming a molecule and the fragment term represented as an explicit function of some basic topological characteristics of the molecular structure. The original mathematical form for description of non-linear contribution is suggested. A five-parameter correlation with the squared correlation coefficient $R^2 = 0.9993$ gives excellent predictions for 168 saturated hydrocarbons, with standard deviation $SD = 2$ K and mean error of ± 1.43 K. All the parameters involved in these equations can be derived solely from the chemical structure.

Key words: QSPR, structural descriptors, hydrocarbons, branching, boiling points

Conducting Properties of Some Biomaterials at Different Temperatures and γ -Irradiation

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The effect of γ -irradiation on the electrical conductivity properties of the biomaterials acrylic resin and silicon rubber was studied. Conductivity data of acrylic resin are mostly unaffected by the exposure of different doses of radiation. The variation in the data of the silicon rubber is due to free radical mechanism, where the electrical conductivity values are decreased with the increase of the dose of γ -radiation. Infrared analysis of acrylic resin before and after γ -irradiation revealed no significant chemical change. The silicon rubber is strongly affected as a result of irradiation.

Key words: biomaterials, conductivity, temperature and γ -irradiation

Transport of Phenanthroline Complexes of Manganese(II) Ions through Nafion Layer on Glassy Carbon Electrode

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Apparent diffusion coefficients of $[\text{Mn}(\text{phen})_2(\text{H}_2\text{O})_2]^{2+}$ and $[\text{Mn}(\text{phen})_3]^{2+}$ in Nafion layer on glassy carbon electrodes were calculated and discussed. Charge transport mechanism was qualified on the basis of voltammetric and coulometric measurements and confirmed by use of the impedance spectroscopy. Electrocatalytic activity against several reductants (glycol aldehyde, glycol acid and ascorbic acid) was examined.

Key words: Mn(III)/Mn(II) couple, formal potentials, modified electrodes, phenanthroline, diffusion coefficients

Synthesis and Characterization of a New Unsymmetrical Porphyrin Liquid Crystal and Its Metal Complexes

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Meso-substituted unsymmetrical porphyrin liquid crystal, 5-(p-palmitoyloxyphenyl)phenyl-10,15,20-triphenyl porphyrin (PPTPPH₂) and relative transition metal complexes (PPTPPM, M = Zn, Co, Mn, Cu, FeCl) were synthesized and characterized by means of elemental analysis, UV-Vis, IR, MS and ¹H NMR spectroscopies. Furthermore, the thermal stabilities and fluorescence spectroscopy of these complexes were investigated. The liquid crystal properties were investigated by differential scanning calorimetry (DSC) and polarized optical microscopy (POM). The results reveal that the PPTPPH₂ shows liquid crystalline behavior with more than one mesophase and it has a low-lying phase transition temperature, which changes from 3.9 to 73.5 °C.

Key words: porphyrin, transition metal, fluorescence spectroscopy, liquid crystal

Evolution of Quantum Similarity Measures: How They Perform in Modeling Hammett Constants

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This study was aimed at comparing a few measures of similarity of carboxylic acids' molecules, based on the electronic descriptors derived from molecular wave functions. Five series of molecules were investigated: benzoic acids, thiophene-2-carboxylic acids, furane-2-carboxylic acids, *trans*-cinnamic acids, and 3-phenylpropionic acids. It has been previously found that instead of comparing densities or other electronic properties of the entire molecules, it is sufficient to use the properties within a molecular fragment, active towards a given reaction. In this vein, three measures have been compared: the one pertaining to the properties of bond critical points, the one derived from atomic potentials, and that based on Fermi-hole densities, confined to the COOH group. Nevertheless, it appeared that other ways of defining a similarity measure may also be practical, namely that based on charges of the COOH group and that based on the properties of another molecular fragment, *i.e.* the substituent and the ring carbon atom connected to the so-called substituent active region. The calculations were carried out at the B3LYP/cc-pVDZ level.

Key words: similarity, substituent active region, atomic electrostatic potential, bond critical point, Fermi hole, carboxylic acids

Fragment-topological Descriptors for QSPR Estimation of Normal Boiling Temperature of Organic Oxygen Compounds

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The new QSPR correlation equation was developed for the estimation of the boiling points of three families of oxygen containing aliphatic compounds. This equation includes contributions depending on the total number of carbon atoms forming a molecule and the fragment term represented as an explicit function of some basic topological characteristics of the molecular structure. The original mathematical form for description of non-linear contribution is suggested. A three-parameter correlation with the squared correlation coefficient $r^2 = 0.9991$ gives excellent predictions for 116 oxygenated compounds, with mean square deviation $s = 2.09$ K and mean error of ± 1.66 K. All the parameters involved in these equations can be obtained solely from the chemical structure.

Key words: alcohols, ethers, aldehydes, ketones, normal boiling points, QSPR

**Investigation of Ozone Synthesis Using a Porous
Emission Electrode in a Coupled Pulsed
Corona Discharge – Surface Discharge System**

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