Synthesis, Spectral and Structural Characteristics of Novel Complex Compounds of Ru(III), Rh(III) and Pd(II) with Typical and Atypical Ways of Coordination of 2-(3-Pyridilmethyliminomethyl)phenol

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Ru(III), Rh(III) and Pd(II) metal complex of a 2-(3-pyridilmethyliminomethyl)phenol with typical and atypical ways of coordination have been synthesized and characterized by elemental analyses, electronic, IR, $^1$H and $^{13}$C NMR spectra, and also by X-ray structure determination for the compounds in crystal form. It has been found that the coordination manner in obtained complexes depend mostly on synthesis conditions.

Key words: Schiff base, metal chelates, adducts, platinum metals
Studies on Schiff Base Complexes of Salicylaldehyde with Sulphamethoxazole and Their Antimicrobial Activities

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New neutral Schiff base complexes of Cu(II), Co(II), Ni(II) and Zn(II) derived from salicylaldehyde and sulphamethoxazole have been synthesized. The structural features of the complexes have been confirmed by microanalytical data, IR, UV-Vis and EPR techniques. The electronic absorption spectra and magnetic susceptibility measurement values of the complexes indicate square-planar geometry for copper and nickel and tetrahedral for cobalt and zinc complexes. The neutral nature of the complexes follows from their low molar conductance values. The EPR spectrum of copper complex in DMSO at 300 K and 77 K was recorded and its salient features are reported. The antimicrobial activity of the complexes has been extensively studied on microorganisms such as Staphylococcus aureus, Bacillus subtilis, Escherichia coli and Pseudomonas aeruginosa by well-diffusion technique using DMSO as a solvent. The values of zone of inhibition were found out at 37°C for a period of 24 h. It has been found that all the studied complexes have higher activity than the free ligand and the standard.

Key words: salicylaldehyde, sulphamethoxazole, Schiff base complexes, antimicrobial activity
Structural and Spectroscopic Characterization of Mixed Ligand Complex: Bis(quinoline-2-carboxylato)bis(imidazole)manganese(II) by D. Dobrzyńska¹, L.B. Jerzykiewicz², J. Jezierska² and E. Słońiec¹

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A new complex, [Mn(quin-2-c)₂(Him)₂] (quin-2-c = quinoline-2-carboxylate ion, Him = imidazole), was synthesized by self assembly and its structure was determined by X-ray analysis. The compound crystallizes in the centrosymmetric space group C2/c with the Mn atom on a twofold axis, \(a = 18.091(6) \text{ Å}\); \(b = 10.125(4) \text{ Å}\); \(c = 13.708(5) \text{ Å}\); \(\beta = 111.73(3)^\circ\); \(V = 2332.5(15) \text{ Å}^3\) and \(Z = 4\) (\(T = 100 \text{ K}\)). Strong hydrogen bonds between imidazole moieties and carboxylate groups connect the molecules of the complex into the 1D chains extending parallel to the \(c\) axis. The interchain contacts of the C–H···O, C–H···N, \(\pi\cdots\pi\) and C–H–\(\pi\) type influence the architecture of the crystal. The complex was characterized by thermal analysis, and by EPR and IR spectroscopy.

**Key words**: manganese, carboxylate ligand, X-ray structure determination, EPR spectroscopy, hydrogen bond
Microcapillary Electrophoresis with Fluorescence Detection

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The advantages and application perspectives for microcapillary electrophoresis (µCE) are presented. The microchip based on a glass plate was fabricated. The separations of three FITC-labeled amino acids carried out with the conventional CE system and in the microchip were compared. The obtained results proved the usability of the microchip for µCE process.

Key words: miniaturization, capillary electrophoresis, amino acids, fluorescence
Synthesis of N,S-Substituted 4-Chloro-2-mercapto-5-methylbenzenesulfonamide Derivatives as Potential Anti-HIV Agents

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A new series of N,S-substituted 4-chloro-2-mercapto-5-methylbenzenesulfonamide derivatives 12–15, 17, 18 and 20–24 have been synthesized as potential anti-HIV agents. All compounds were screened at the National Cancer Institute (Bethesda, USA) for their in vitro anti-HIV-1 activity, and relationships between structure and anti-HIV activity are discussed. The prominent compounds with remarkable activity were 22 (EC50 = 5.9 μM) and 24 (EC50 = 5.1 μM).

Key words: N,S-substituted 4-chloro-2-mercapto-5-methylbenzenesulfonamides, synthesis, anti-HIV activity
Activation of
N-Benzoyl-2-substituted-2-hydroxymethyl-2-amino
Acids with Chiral Coupling Reagents Prepared in situ
from 2-Chloro-4,6-dimethoxy-1,3,5-triazine

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Chiral triazine condensing reagents were obtained in situ by treatment 2-chloro-4,6-dimethoxy-1,3,5-triazine with strychnine, brucine, sparteine, nicotine and quinine, and used for enantioselective activation of racemic N-benzoyl derivatives of 2-methylserine, 2-isobutylserine and 2-benzylserine affording enantiomerically enriched appropriate 2-phenyl-4-hydroxymethyl-4-substituted-1,3-oxazolin-5-one. Configuration and ee of products were determined by HPLC on chiral stationary phase. S configuration of enantiomer activated faster to oxazolinone was confirmed for all chiral amines except quinine. For the later amine, R enantiomer of N-benzoyl-2-methylserine was activated faster. For experiments involving strychnine as chiral auxiliary, enantiomeric enrichment was substantially lower than in the case of proteinogenic amino acids and increased with the size of Cα-substituent from 12% ee for methyl to 36% ee for isobutyl side chain.

Key words: 2-methylserine, 2-isobutylserine, 2-benzylserine, enantioselective activation, 2-chloro-4,6-dimethoxy-1,3,5-triazine
The Reaction of Tris(aminoethyl)amine with Rigid Aromatic Dialdehydes as a Convenient Tool for the Synthesis of Cryptands

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Four bicyclic octaaza cryptands and three triaza macrocyclic amines have been synthesized via the reaction of tris(aminoethyl)amine with six rigid aromatic dialdehydes, followed by reduction of the formed Schiff bases with sodium borohydride.

Key words: imination reaction, Schiff bases, macrocycles, cryptands
Spectroscopic $^1$H NMR, $^{13}$C NMR and Theoretical DFT Study of Isoguanine and 8-Oxoadenine in Water and DMSO-d$_6$ Solutions

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$^1$H and $^{13}$C NMR spectra of isoguanine (2-hydroxyadenine) and 8-oxoadenine in H$_2$O and DMSO-d$_6$ solutions of various acidity have been interpreted using arguments based on the results of several 1D and 2D NMR experiments and theoretical DFT-based calculations. The collected data for H$_2$O solutions can serve for identification of these compounds in body fluids during medical analysis. The $^1$H and $^{13}$C NMR spectra of the investigated compounds in DMSO-d$_6$ solutions have provided information on their tautomeric forms and the mobility of their exchangeable protons.

Key words: isoguanine, 8-oxoadenine, tautomerism, protonation, $^1$H NMR, $^{13}$C NMR
Gold Nanoparticles from Oxonium Precursor: Synthesis in the Presence of Primary Amine and Characterization

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A convenient method of the synthesis of gold NPs with low polydispersity is described. Triphosphinogold oxonium salt $[O(AuPPh_3)_3]BF_4$ in the presence of amine and dioxygen is a versatile gold atom source in mesitylene. The amine takes part in the reduction of gold(I) atom precursor. Therefore in a 1/1 Au(I)/hexadecylamine stchiometry, “naked” gold nanoparticles are produced which precipitate within some minutes from the solution and form a gold mirror. Only an excess of amine enables the synthesis of ligand-protected nanoparticles which furthermore display a great tendency to self-organize. Solvent effect on the course of the reaction is discussed.

Key words: gold, nanoparticles, synthesis, aggregates
Theoretical Study on the Chemical Reactions in the Cl-ClO Catalytic Cycle

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One of the processes of ozone depletion in the polar stratosphere was investigated using ab initio calculations at the MP2, B3LYP, QCISD(T), G2, G2MP2 and CBS-Q levels. The reactional energy, the enthalpy of formation, and the relative Gibbs free energy of the reactions in the Cl-ClO catalytic cycle were calculated. The energies of the transition states of the reactions were calculated, followed by the calculations of the reaction barriers. The results support the mechanism of ozone depletion by the Cl-ClO catalytic cycle, and explain the basic reason of ozone depletion from the point of energy.

Key words: ozone depletion, Cl-ClO catalytic cycle, ab initio calculations, energy
Ionization of Organic Acids in Dimethyl Sulfoxide Solution: Different Methods of the Ab Initio Calculation of the pKₐ Using the Polarizable Continuum Model

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The pKₐ values of ten organic acids in dimethyl sulfoxide (DMSO) solution were calculated using the density functional theory (DFT), second-order Moller-Plesset Perturbation (MP2) and Hartree-Fock (HF) methods at the 6-31+G(d) basis set level. The solvation was included through the polarizable continuum model (PCM). The major work was to compare the different PCM methods to calculate the pKₐ, as well as coupled with the experimental data. The average error over this set of molecules using the HF method is smaller than those using B3LYP or MP2 methods, not only in theoretical calculation but also in the mix approach (coupled with the experimental data). The present result suggests that the HF method in PCM model could be used for predicting the pKₐ values.

Key words: density functional theory, pKₐ, DMSO, PCM
n-Pentane and 3-Methylpentane Conversions on Differently Pretreated Supported Palladium Catalysts
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Metal-support interactions in silica- and alumina-supported palladium catalysts have been investigated by using n-pentane and 3-methylpentane conversions as test reactions. High temperature reduction (HTR) at 600°C results in a considerable increase of the selectivity towards isomeric and cyclic products, i.e. causes a similar effect as in the case of previously studied reactions of 2,2-dimethylpropane and various C₆-alkanes. However, the silica-supported palladium catalysts behave differently from the Pd/Al₂O₃. For the former catalysts subjected to HTR, the selectivity for cyclic products is enhanced, whereas a similarly pretreated Pd/Al₂O₃ gives mainly isomers. This observation, and the changes in both the hydrogen reaction order and in the activation energy caused by different catalyst pretreatment, were both analyzed in detail. All mentioned quantities appeared to be new convenient diagnostic parameters towards determining whether or not palladium interacts with a support.

Key words: n-pentane, 3-methylpentane, catalytic conversion of, Pd/Al₂O₃, Pd/SiO₂, effect of catalyst pretreatment, isomerization selectivity, hydrogen reaction order
Electrochemical Deposition of W–O–Se Thin Films on Polycrystalline Pt Electrode

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The possibility of electrochemical deposition of W- and Se-containing thin films on polycrystalline Pt electrode is demonstrated. Various electroanalytical techniques (linear sweep and cyclic voltammetry, chronopotentiometry, chronoamperometry) were used for the elucidation of some peculiarities of deposition process. An acidic electrolyte composed of selenious acid and tungsten(VI) peroxo complex in 0.3 M nitric acid was used for the synthesis. It was established that the as-deposited W–O–Se layers are amorphous and contain various amounts of tungsten and selenium, depending on synthesis conditions.

Key words: electrochemical reduction, electrodeposition, selenious acid, tungsten
Photoconducting Properties of Fullerene Derivatized with a Biphenyl Moiety

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The properties of low molecular weight molecules, in which the electron-acceptor fullerene unit was linked by malonate group and flexible long alkyl chains to two biphenyl-phenyl units, were studied. Cyclic voltammetry measurements showed five consecutive one-electron, reversible electro-reductions for the fullerene unit and a single two-electron, reversible electro-oxidation for biphenyl moiety. The two electron process indicated that two biphenyl moieties interacted; presumably folded conformation was formed with two electron donating moieties at close proximity. A long-living charge-separated state induced upon light absorption was confirmed by the ESR spectroscopy studies. These properties were responsible for observed photoconductivity of the studied compound.

Key words: fullerene, photoconductivity
Synthesis, Crystal Structure and Magnetism of 1D Manganese(II) Coordination Polymer with Thiocyanato as Bridging Ligand

by J.-M. Shi, J.-N. Chen and L.-D. Liu

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The Reversible Reaction of 2,5-Diformylfuran with Primary $\alpha,\omega$-Diamines – an Interesting and Useful Process for Dynamic Combinatorial Chemistry

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Thiophene Hydrodesulfurization over Ni-Mo Catalysts Supported on Graphitized Active Carbons

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