Synthesis and Characterization of Cu(II), Co(II), Ni(II) and Zn(II) Schiff Base Complexes from 1-Amino-5-benzoyl-4-phenyl-1H-pyrimidine-2-one with Salicylaldehyde

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Cu(II), Co(II), Ni(II) and Zn(II) metal complexes of new heterocyclic Schiff base derived from 1-amino-5-benzoyl-4-phenyl-1H-pyrimidine-2-one with salicylaldehyde have been synthesized and characterized by elemental analyses, mass, electronic, IR and ¹H NMR spectra, and also by molar conductivity measurements, magnetic moment measurements and thermogravimetric analyses (TGA). It has been found that the Schiff bases behave as a neutral bidentate (NO) and tridentate (ONO) ligands forming chelates with 1:2 (metal:ligand) stoichiometry. Octahedral environment is suggested for metal complexes. The conductivity data for the Ni(II) complexes are consistent with those expected for an electrolyte.
Phase Equilibria in the AgGaS$_2$–GeS$_2$ Systems

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The AgGaS$_2$–GeS$_2$ section has been investigated using the methods of physico-chemical analyses. The existence of $\alpha$-tetragonal, $\beta$-monoclinic solid solutions on the basis of the initial compounds and the intermediate $\gamma$-phase, which crystallizes in Fdd2 space group, has been established. The $\gamma$-phase forms the eutectics with the initial components. Their coordinates are: 42 mol.% GeS$_2$ (1121 K) and 93 mol.% GeS$_2$ (1095 K).
The reaction of cholesteryl acetate with ozone in the presence of amines has been studied. Besides the expected cleavage products, B-seco-ketoaldehyde and its aldol condensation product, 5-hydroxy-6-formyl-B-nor-5β-cholestane derivative, the abnormal product, 3β-acetoxy-A-nor-3(5→6α)abeo-6β(H)-cholestan-5-one is formed as a result of a new, anomalous cleavage of the primary ozonide. The reaction conditions and isolation procedure were optimized for achieving good yield of the abeo-compound. The X-ray crystal structure analysis confirmed the formation of the unusual steroidal skeleton. It appears to be the first crystallographic analysis of the transformed steroid with A-nor-3(5→6α)abeo skeleton. No product resulting from the amine nucleophilic participation in the cleavage of ozonides was observed.
New Chromogenic Azothiacrown Ethers –
Synthesis and Properties

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New chromogenic azocrown ethers possessing sulfur atoms and two azo- groups in the macrocycle are described. The synthesized macrocycles have been applied as ion carriers in ion-selective membrane electrodes. Their selectivity and sensitivity were studied towards alkali and transition metal cations. Complexation of the compounds was studied by UV-Vis spectrophotometry in water–dioxane (1:1; v/v) solvent system. Stability constants of copper and silver complexes were determined. Contrary to oxygen analogues, the azothiacrowns do not form complexes with alkali or alkaline earth metal cations.
Syntheses of \( N\)-aryl-\( N'\)-(4-chloro-2-alkylthio-5-methylbenzenesulphonyl)guanidines with Potential Biological Activity

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Syntheses of new \( N\)-aryl-\( N'\)-(2-alkylthio-4-chloro-5-methylbenzenesulphonyl)guanidine 3–14 are described. The facile conversion of 1 and 8 to new 2-[(2-amino-6-dimethylamino-1,3,5-triazin-4-yl)methylthio]benzensulphonylcyanamide 16 and 2-[(2-amino-6-dimethylamino-1,3,5-triazin-4-yl)methylthio]benzensulphonylguanidine 17 respectively, was elaborated. The preliminary anticancer evaluation of 16, 17 was performed at US National Cancer Institute.
1-(N,N-Dimethylamino)-2-(N-phenylcarbamoyl)-1-buten-3-one as a Building Block for the Synthesis of Heterocyclic Compounds

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Acetoacetanilide I reacted with DMF-DMA to give the enaminone 2. Compound 2, when treated with hydrazines gives the pyrazoles 4a and 4b respectively, and with pyrazole derivatives 5a and 5b the pyrazolopyrimidines 7. On the other hand, in reaction of 2 with benzimidazole and benzimidazole-2-acetonitrile, the pyrimidobenzimidazole 14 and the pyridobenzimidazole 17 were formed. 2 reacts with hippuric acid in boiling acetic anhydride to afford the pyridine 20. In the reaction of 2 with malononitrile, cyanoacetamide or malononitrile dimer compounds 21, 22 and 24 were formed. Compound 22 was further reacted with arylidenemalononitriles to give the benzopyridine derivatives 28. Pyridone 22 treated with S-DMF mixture gives thienopyridine 29, while refluxed with DMFDMA yielded the pyridopyridine 30.
The Reactions of 2-(Chloroseleno)benzoyl Chloride with Pyridine and Related Azines

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The reaction of 2-(chloroseleno)benzoyl chloride with pyridine and pyridine-like heterocycles such as pyrimidine, pyrazine, quinoline, phthalazine, phenazine and 1,10-phenanthroline was studied. In the most cases stable 2-(hydroxyseleno)benzyazinium chlorides were produced depending on the number of the pyridinium-like nitrogen atoms and their situation in the ring system.
Synthesis of 1,3-Dideoxynojirimycin via an α-Amino Aldehyde as a Key Intermediate

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1,3-Dideoxynojirimycin was synthesized starting from a suitably protected α-amino aldehyde. The crucial step involves addition of allyl bromide to N-benzyl-N-carbo-benzoxy-O-tert-butyldimethylsilyl-D-serinal in the presence of tin(II) chloride and sodium iodide.
Flavonoids from the Leaves of *Prunus spinosa* L.

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Two new flavonol glycosides, quercetin 3-O-(2''-O-β-D-glucopyranosyl)-α-L-arabinofuranoside and kaempferol 3-O-(2''-O-E-p-coumaroyl)-α-L-arabinofuranoside-7-O-α-L-rhamnopyranoside, were isolated from the leaves of *Prunus spinosa* L. The known compounds, kaempferol, quercetin, and their 3-arabinofuranosides, kaempferol 7-rhamnopyranoside, kaempferol 3,7-dirhamnopyranoside, and kaempferol 3-arabinofuranoside-7-rhamnopyranoside were also identified. Structural elucidation was performed by means of chemical methods and UV, IR, LSI MS, 1D and 2D NMR spectroscopy.
Sulfonation of the Naphthalene Derivatives in Protic Solvent. Principles of Isomer Distribution

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The principles of formation of mono- and disulfonation products of selected derivatives of naphthalene in protic solvents were studied. The position of electrophilic substitution was compared with: localization energies (\(L^+\)) of the parent compounds; steric effect of methoxy groups; partial charges on carbon atoms in aromatic ring; dipole moment (\(\mu\)) and the binding energies of the products (D). These results suggest that only steric hindrance and the binding energy of the sulfonation products of naphthalene derivatives in protic solvents may be a good prognostic index for isomer distribution substitution products.
Adsorption Behaviour of Laprol 2402 C on Copper Electrode

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Voltammetry and EIS were applied to study the adsorption behaviour of laprol 2402 C (the copolymer of ethene and propene oxides) on a Cu electrode in strongly acidic Cu(II) sulphate solutions. Analysis of impedance data was carried out on the basis of adequate equivalent circuits, containing electric analogues of the electrochemical system. The results indicate that laprol displays a rather weak surface activity on copper in chloride-free solutions. Pronounced inhibition of Cu(II) reduction takes place, when micromolar amounts of chloride are added. A more compact surface layer involving Cl⁻ ions is thought to be formed under these conditions.
Electronic structure calculations based on the density functional theory (DFT) have been applied to the adsorption of hydrogen on the (100) plane of TiH₂. Calculations have been performed for a supercell of TiH₂ and the periodic boundary conditions have been used. Three different monolayers, two double layers and one selected submonolayer of hydrogen have been considered. It is shown that the most dense coverage corresponds to a submonolayer composed of atoms in the bridge position with respect to titanium atoms on the surface. Both, binding energy and the hydrogen density on the surface agree with the experimental results.
Study of the Inclusion Complexes of Catecholamines with β-Cyclodextrin by Cyclic Voltammetry

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The inclusion complexes of catecholamines (dopamine, DA, and adrenaline, AD) with β-cyclodextrin (β-CD) have been studied by cyclic voltammetry (CV) using glassy carbon electrode (GCE) for expanding the potential window. The variations of peak potential and peak current were observed on cyclic voltammograms, when the electroactive guest molecules, DA and AD are complexed with β-CD. Dissociation constants of cyclodextrin inclusion complexes have been calculated. The experimental results indicate that both DA and AD can form a 1:1 inclusion complexes with β-CD in aqueous solutions. It was observed that the light and oxygen sensitivity of the inclusion complex is much lower than those of the free catecholamines, which can be used to improve their storage and handling, and also widen their applications in pharmaceutical industry. Furthermore, it was found that their electrochemical oxidation in the aqueous solutions could be inhibited by β-CD.
Isotopic rate constant ratios, $k_{14}/k_{15}$, have been determined for the decomposition of nitric oxide over copper wire at initial NO pressures 40–60 kPa over temperature range 725–825 K. They were interpreted using the Bigeleisen formalism. Under these experimental conditions the reaction was found to be second order in NO. On the basis of the temperature independence, $k_{14}/k_{15} = 1.010 \pm 0.001$ at all temperatures studied, a *cis* ONNO transition state was shown to account satisfactorily for the experimental $k_{14}/k_{15}$ values.
The Limited Penetration Depth of Nickel Hydride at 298 K

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At three different gaseous hydrogen pressures (7.65; 10.26 and 12.36 kbar) the penetration depth of nickel hydride was determined in stationary conditions at 298 K, increasing from 35.5 $\mu$m to 59.5 $\mu$m and being a linear function of the ln of hydrogen fugacity. At the above temperature 30 $\mu$m is the minimal penetration depth of nickel hydride. Kinetic reasons are supposed to be responsible for the limited penetration depth.
Variations of Tautomeric Preferences in Histamine Monocation – Ab initio Studies for “Essential” and “Scorpio” Conformations from the Gas Phase to Aqueous Solution

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The polarizable continuum model (PCM) for geometries optimized at the RHF/6-31G* was applied to study the variations of the tautomeric preferences in the histamine monocation from the gas phase to aqueous solution. Seven solvents of different polarities (from cyclohexane to water) were chosen and calculations performed. A change of the tautomeric preference takes place already in apolar solvents containing heteroatoms. The ring N-aza protonated form (ImH+) is only favoured in the gas phase and cyclohexane, benzene, CCl₄. The chain N-amino protonated form (AmH+-T₁) predominates in other solvents: CHCl₃, THF, acetone, water.
Catalytic Ketonisation over Oxide Catalysts. Part V. Synthesis of Cyclopentanone over MnO$_2$/Al$_2$O$_3$ Catalysts

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Dicopper(II) with Ferromagnetic Coupling, Antiferromagnetic Dimanganese(II) Complexes Containing 3-Nitro-phthalato as Bridging Ligand: Synthesis and Magnetism

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Complexes of Zinc(II) and Cadmium(II) with Bipyridine Isomers and Monohalogenoacetates

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