The Crystal and Molecular Structure of 1-Methyl-4-(p-methylbenzylidene)-2-methylseleno-5-imidazolinone

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The crystal structure of 1-methyl-4-(p-methylbenzylidene)-2-methylseleno-5-imidazolinone has been determined by X-ray diffraction methods. The crystals are triclinic, space group $P\overline{1}$, with $a = 8.130(1)$ Å, $b = 8.888(1)$ Å, $c = 9.287(1)$ Å, $\alpha = 93.80(1)^\circ$, $\beta = 94.86(1)^\circ$, $\gamma = 92.67(1)^\circ$, $Z = 2$. The molecule is approximately planar with most of the bonds participating in a conjugated system, stabilized by weak intramolecular hydrogen bond, C8–H8\cdot\cdot\cdotN1. Conclusions about electron distribution within this system have been drawn from the bond angles and bond lengths. In the unit cell, molecular pairs can be discerned with antiparallel imidazole rings in the distance of 3.5 Å.

Synthesis and Biological Activity of New Diarylalkenes

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Condensation of 5-nitro-, 3-chloro-, and 5-chlorosalicylic acids with formaldehyde afforded dimeric disalicylmethanes, which were $O$-methylated with dimethyl sulfate and oxidized with chromium(VI) oxide to diarylketones 9, 10, 11, 12. Wittig reaction with ylides obtained by deprotonation of alkyltriphenylphosphonium salts with sodium bis(trimethylsilyl)amide yielded a series of diarylalkenes. Some of the obtained compounds showed high antibacterial activity in vitro against Erwinia carotovora.

Synthesis and Properties of Azoles and Their Derivatives. XLIII. Regio- and
Stereoselectivity of [2+3] Cycloaddition Reaction of E-β-Nitrostyrene to Z-C-Aryl-N-phenylnitrones

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E-β-Nitrostyrene (1) reacts with Z-C-aryl-N-phenylnitrones (2a–h) exclusively to give trans- and cis-2,5-diphenyl-3-aryl-4-nitroisoxazolidines (3a–h, 4a–h) in high yield. The molar ratio of trans and cis stereoisomers is affected by substituent in phenyl ring of the parent nitrone (2e) The reaction is found by AM1 calculations to be controlled by the interactions of the HOMO of nitrone with the LUMO of nitrostyrene.


Reaction of (+)-3-Carene and (+)-2-Carene with t-Butyl Hypochlorite or N-Chlorsuccinimide in the Presence of Free Radical Catalysts

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Allylic chlorination of (+)-3-carene (1) gave (−)-trans-4-chloro-3(10)-carene (2), (+)-10-chloro-carene (4) and 3,4-dichlorocarane (5). Chlorination was done by two methods: with t-butyl hypochlorite or N-chlorsuccinimide in the presence of catalytic amount of α,α’-azobisisobutyronitrile or benzoyl peroxide, UV irradiation and silica gel. Chlorination of (+)-2-carene (7) using these methods gave p-cymene (8), 1-isopropylene-4-methylbenzene (9) and dipentene (10).


On the Route to the N-Phosphoryl Sulfamic Acid

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Synthesis of the previously unknown \( N \)-diethyl phosphorosulfamate 15 was accomplished by direct sulfamation of diethyl phosphoroamidate 4 with sulfur trioxide–DMF complex 14. The acid 15 was isolated in form of benzyl–16 and cyclohexylammonium 17 salts, which were found to be unstable in water solution. The other possible routes to sulfamate 15 were briefly tested.


**Kinetics and Mechanism of Oxidative Transformations of (6R)-6-(\( \alpha \)-Phenyl-D-glycylamino)penicillanic Acid (Ampicillin) by Manganese(III) in Pyrophosphate Medium**

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Manganese(III) has been stabilized in weakly acidic solution by pyrophosphate and the complex formed was elucidated spectrophotometrically. Stoichiometry of manganese(III) oxidation of ampicillin in pyrophosphate medium was established in the pH range 2.0–3.0 by iodometric and spectrophotometric methods. The oxidation follows first order kinetics in \([\text{Mn(III)}]\). The effect of varying \([\text{Mn(III)}], [\text{Amp}], [\text{H}^+]\), added \([\text{Mn(II)}]\), total \([\text{P}_2\text{O}_7]^{4-}\) and added \([\text{ClO}_4^-], [\text{SO}_4^{2-}]\) ions have been studied. The order in \([\text{Amp}]\) is unity and increase in \([\text{H}^+]\) increases the rate. With increase in \([\text{Mn(II)}]\) and \([\text{P}_2\text{O}_7]^{4-}\), a retardation effect was noticed. Oxidation products have been proposed. Dependence of reaction rate on temperature has been studied and activation parameters were computed. A mechanism consistent with the observed results has been proposed.


**Physico-Chemical Characteristics of Sulfated Mixed Oxides of Sn with Some Rare Earth Elements**

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A series of binary mixed oxides of tin with three rare earth elements viz. La, Ce and Sm were prepared by co-precipitation method and sulfate treatment was performed by treating the mixed hydroxides with sulfuric acid or ammonium sulfate. The physicochemical characterization has been done by XRD, BET-SA, SEM, EDX, TG-DTA and IR spectroscopy. Adsorption of n-butylamine was used to probe the acidic properties of the catalysts. The strength and distribution of acid sites depend on the mixed metal oxide composition, as well as on the preparation method. The rare earth modified sulfated tin oxide catalysts are more active in the oxidative dehydrogenation of cyclohexanol and cyclohexane, compared to the corresponding mixed oxide systems and sulfated tin oxide. Among the different sulfated oxide systems investigated, cerium promoted catalysts displayed a better selectivity towards dehydrogenation products.


Stability and ESR Spectra of Ni(III) Tetraazamacrocyclic Complexes in Nitrate and Chloride Solutions

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Complexes [NiIII(cyclam)Cl2]Cl (1), [NiIII(cyclam)(NO3)2]ClO4 (2) and [NiIII(2-methyl-cyclam)(NO3)2]ClO4 (3) were isolated and the stability of Ni(III) was studied by UV-VIS spectrophotometry as a function of NaCl and NaNO3 concentration. In complexes 2 and 3 the decay of Ni(III) followed the first order kinetics in aqueous and in nitrate solutions up to 1 mol/dm³. In complex 1 the first order kinetics was observed only in aqueous and saturated NaCl solutions. With increase in NaNO3 concentration the stability of Ni(III) in complexes 2 and 3 increased however, in complex 3 it was lower than in complex 2. Stability of Ni(III) in complex 1 increased also with increasing NaCl concentration but it diminished starting from 2 mol/dm³ NaCl. The forms of complexes depending on the salt concentration were characterized by the ESR technique.


Structure and Hydrogen Bonding of Solid N¹-Alkyl-N²-(2-hydroxy, 4- or 5-methylphenyl)thioureas

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Crystalline N1-alkyl-N2-arylthioureas with ortho hydroxyl and para or meta methyl substituents to the phenyl ring were studied by single crystal X-ray diffraction, IR and solid state 13C CP MAS NMR. Two different modes of association were found: i) intermolecular N1H...S bonds and N2H not involved in hydrogen bonding in N1-methyl-N2-(2-hydroxy,5-methylphenyl)thiourea 1, ii) cyclic dimers with two N2H...S hydrogen bonds (S...N2 distance of 3.322 Å) and N1H engaged in intermolecular N1H...O bond in N1-methyl-N2-(2-hydroxy,4-methylphenyl)thiourea 2. Changes of carbon chemical shifts between solution and solid state result mainly from the reorientation of the aromatic ring with respect to the thiourea fragment.


Synthesis of a New Triazine Derived Macrocycle and a Thermodynamic Study of Its Complexes with Some Transition and Heavy Metal Ions in Acetonitrile Solution


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A synthetic procedure has been developed for the preparation of a new triazine derived macrocycle ([13,29-diphenyl-4,7,20,23-tetraoxa-1,10,12,14,16,17,26,28,30,32-decaaza-[10,10](2,6)triazinophane]. The formation of some transition and heavy metal complexes with the macrocycle was investigated in acetonitrile solution conductometrically at different temperatures. The formation constants of the resulting 1:1 complexes were determined from the molar conductance-mole ratio data and found to vary in the sequence Hg2+ > Pb2+ > Cd2+ > Ag+ > Cu2+ > TI > Co2+ > Ni2+ > Zn2+. The enthalpy and entropy of complexation reactions were determined from the temperature dependence of the formation constants. In all cases, the complexes were found to be enthalpy stabilized but entropy destabilized.
Characterization of Polyacetylene and Polyacetylene Doped with Palladium


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Samples of Naarmann polyacetylene, denoted as N-(CH)x, (unstretched) and polyacetylene doped with Pd have been investigated, being characterized by: (i) conductivity using the four-point method, (ii) bulk concentration of Pd using the atomic absorption method, (iii) bulk density using helium pycnometry, (iv) surface composition by X-ray photoelectron spectroscopy and (v) electron transport parameter, such as the inelastic mean free path, using elastic peak electron spectroscopy. For evaluating the inelastic mean free path, a Ni standard has been applied, using three spectrometers in the electron energy range 200–5000 eV. The experimental values of the inelastic mean free path have been compared with that obtained earlier by Tanuma et al. for Shirakawa polyacetylene and with that resulting from the TPP-2M predictive equation and the G1 predictive formula of Gries. The scatter between the experimental and theoretical inelastic mean free path values has been discussed. The experimental inelastic mean free path values depend on the density of the polymers and the surface composition, associated with the contamination from the reaction synthesis.

Synthesis and Magnetic Properties of Tetranuclear Copper(II)–Cobalt(II) Complexes of Macrocyclic Oxamides

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In-situ Spectroelectrochemical Investigation of Inclusion Complex of Pyrocatechol and Cyclodextrin in Poly(pyrrole) Film

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The Crystal Structure of Monoaquabis(trans-5-methylpyrazine-2-carboxylato-N,O)copper(II) Trihydrate

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Ternary Liquid – Liquid Equilibria: Hexamethyldisiloxane – Dimethyl Sulfoxide – Methyl Ethyl Ketone (-Diethyl Ketone)

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Ni(PzBu-t)4(N3)2 – a Versatile Precursor as Ligand for the Design of the Heteropolymetallic Systems
IUPAC RECOMMENDATIONS ON NOMENCLATURE AND SYMBOLS

Physical Chemistry Division
Commission on Colloid and Surface Chemistry Including Catalysis

Nomenclature of Structural and Compositional Characteristics of Ordered Microporous and Mesoporous Materials with Inorganic Hosts