

Krešimir Furić

Depolarization Ratio ρ_{\perp} ($\pi/2$) of Raman Bands for Dissolved and Molten Benzoic Acid Dimers

Conformation of benzoic acid dimers in the solution and in the melt is examined using Raman spectroscopy. The number of observed depolarized bands does not agree with the generally accepted assumption on dimers' planarity. . . .

1—6

Nevenka Pavković,
Biserka Kojić-Prodić,
Milenko Marković,
and Dejan Plavšić

Precipitation and Characterization of Strontium Phosphates

The spontaneous precipitation of strontium phosphates at 298 K and 310 K ($[\text{NaCl}] = 0.15 \text{ mol dm}^{-3}$, $\text{pH}_{\text{init}} = 7.4$) has been studied. Solid phases SrHPO_4 , $\text{Sr}_{10}(\text{PO}_4)_6(\text{OH})_2$, $\text{H}_3\text{Sr}_6(\text{PO}_4)_5 \cdot 2 \text{H}_2\text{O}$ and $\text{Na}[\text{Sr}(\text{H}_2\text{O})_9]\text{PO}_4$ were determined. The value of solubility product of $\text{Na}[\text{Sr}(\text{H}_2\text{O})_9]\text{PO}_4$ is calculated: $\log K_s = -9.98 \pm 0.11$ (at $I = 0.25 \text{ mol dm}^{-3}$, 298 K). . . .

7—15

Željko Kurtanjek

Mathematical Model of the Oscillatory Oxidation of Hydrogen on Nickel

Simultaneous oxidation and reduction of nickel is considered as the cause of oscillatory behavior. The process is investigated by the CPD measurements under the reaction conditions. The model predictions are in semiquantitative agreement with the experimental data. . . .

17—27

Tomislav P. Živković

Molecular Orbital Resonance Theory: Matrix Elements of One-particle Operators

In the Molecular Orbital Resonance Theory (MORT) each resonance structure is defined as an antisymmetrised product of

mutually disjunct bond orbitals. In the present paper expressions for overlaps and matrix elements of one-particle operators between MORT resonance structures are derived.

29—52

**Halka Bilinski and
Nevenka Brničević**

Precipitation and Complex Formation of Zirconium(IV) with Malonic, Succinic and Adipic Acids at 298 K

The precipitation of zirconium(IV) from aqueous solution of zirconyl chloride was investigated in the presence of dicarboxylic acids: malonic, succinic and adipic. In the precipitation diagram only one region at $\text{pH} < 2$ exists in which zirconium is water-soluble with these acids. Polymeric, insoluble compounds of the composition $\text{Zr}(\text{OH})_3\text{HA}$ (A = malonate, succinate, adipate ligands) were isolated at $2 < \text{pH} < 3$.

53—59

**Mladen Biruš,
Zdravko Bradić,
Nikola Kujundžić,
and Marijan
Pribanić**

Kinetics and Mechanism of Interactions Between Iron(III) and Desferrioxamine B. The Formation and Hydrolysis of Ferrioxamine B in Acidic Aqueous Solution

The kinetics of the formation and hydrolysis of ferrioxamine B complexes have been studied in acidic aqueous solution (0.001—1.0 M HCl) at 25.0 °C, $\mu = 1.0$ M (maintained by NaCl). Two stage kinetics have been observed in both the formation and in the hydrolysis reactions. The proposed reaction model involves formation/hydrolysis of bidentate, tetradentate, and hexadentate bonded desferrioxamine B to iron(III).

61—77

**Nenad Raos and
Vladimir Simeon**

Conformational Analysis of Bis-(N,N-dimethylvalinato)copper(II): a Possible Explanation of the Enantioselectivity Effect

The conformational space of the stereoisomers of bis-(N,N-dimethylvalinato)copper(II) was investigated by the consistent force field (CFF) method. The calculated enantioselectivities, defined as Gibbs ener-

gy differences between $M(L\text{-ligand})_2$ and $M(L\text{-ligand})(D\text{-ligand})$ complexes, qualitatively agree with the experimentally observed values.

79—85

**Boris Kamenar,
Dubravka Matković,
and Antun Nagl**

Crystal and Molecular Structure of Two (phenylsulfonyl)-3-(hexahydroazepin-1-yl)-ureas: (A) 1-(4-chlorophenylsulfonyl)-3-(hexahydro-1*H*-azepin-1-yl)-urea and (B) 1-(4-methylphenylsulfonyl)-3-(hexahydro-1*H*-azepin-1-yl)-urea

Crystal structures of title compounds have been determined by X-ray diffraction method. Molecules of (A) and (B) have similar but not identical shape. The hexahydroazepine ring of (B) has a boat conformation while that of (A) is disordered.

87—95

**V. Verma, S. Kher,
and R. N. Kapoor**

Reactions of Hafnium Tetrachloride with Benzoyl Hydrazones

The reactions products of hafnium tetrachloride with monofunctional bidentate and bifunctional tridentate benzyl hydrazones of the type $HfCl_3(BHy)$, $HfCl_2(BHy)_2$ and $HfCl_2(BHy)'$ have been characterized on the basis of elemental analysis, electrical conductance and spectral data.

97—102

**Him-Tai Tsang
and Wai-Kee Li**

**MINDO/3 Study of Cyclopentadienyli-
dene and Its Insertion into Molecular
Hydrogen**

It is found that the ground state of cyclopentadienyli-
dene **1** is a spin triplet. This is in accordance with experimental findings and previous calculations. The least-motion and non-least-motion paths and the molecular hydrogen insertion of **1** are studied. The latter is to be preferred energetically.

103—112

Danilo Dobčnik

**Electroanalytical End-Point Indication
in Hydrolytic Potentiometric Precipitation
Titration by means of the Glass
Electrode**

The hydrolytic potentiometric precipitations titrations of Ba^{2+} with CrO_4^{2-} and vice versa CrO_4^{2-} with Ba^{2+} ions are described.

113—116

Rajeev Jain

Polarographic Investigations of Some 2-Arylazo-2-bromo-5,5-dimethylcyclohexane-1,3-diones

Polarographic behaviour of methyl, methoxy, chloro, bromo and ethoxy derivatives of 2-arylazo-2-bromo-5,5-dimethylcyclohexane-1,3-diones have been examined. The effect of substituents has been interpreted in terms of the Hammett equation.

117—123

Vinko Škarić and Milan Jokić

Homologation and Intramolecular Cyclisation Reactions in Aliphatic Deoxyuridine Analogues Series

The elongation of 1-(2,3-dihydroxypropyl)uracil (I) into 1-(2,4-dihydroxybutyl)homologue was described. The intramolecular transformations of suitably activated I afforded the corresponding derivatives of 2,3-dihydro-2-hydroxymethyl-7H-oxazolo[3,2-a]-pyrimidin-7-one.

125—139

Miće Kovačević, Jure J. Herak, and Branimir Gašpert

Activation of the Carboxylic Acids by Anhydride Formation with *N*-Acyl-*N*-alkyl Carbamic Acid

Preparation of aminosubstituted beta-lactam antibiotics by acylation of 6-APA or 7-ADCA with *N*-protected phenylglycine activated in form of mixed anhydride with *N*-acyl-*N*-alkyl carbamic acid.

141—155

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