Synthesis of Glucuronic Esters of Amino Acids

G. Roglić

»Ruder Bošković« Institute, 41000 Zagreb, Croatia, Yugoslavia

1-O-Acylaminoacyl- and aminoacyl- derivs. of fully methylated glucuronic acid were synthesized and completely characterized by phys. and chem. methods.

The cyclic structure and anomic configuration of methyl 2,3,5-tri-O-methyl-n-glucuronate — the sugar component of these esters — was deduced from NMR spectra, GLC analysis, and the crysat. derivs.

Fully protected glucuronic esters of amino acids were obtained as anomic mixts. in high yields by two methods involving direct participation of imidazole: (a) accelerated active ester (AAE) synthesis and (b) dicyclohexylcarbodi-imide (DCC) condensation. In both reactions the intermediate N-acylimidazole, formed by the nucleophilic attack of imidazole on the activated amino acid ester and the O-acylurea, respectively, participates directly in the transfer of the acyl group to the sugar component. The anomeric sep. of methyl 1-O-acylaminoacyl-2,3,4-tri-O-methyl-n-glucofuranuronates was achieved by column chromatography on silica gel. Both methods proceeded without racemization of the aglycone moiety.

Catalytic hydrogenation of β-anomers of some 1-O-(N-benzyloxy-carbonyl-aminoacyl)-2,3,5-tri-O-methyl-n-glucofuranuronates gave the corresponding 1-O-aminoacyl derivs. which were isolated as mono-oxalate or as internal salts.

For comparison purposes, some compds. from the class of glucose-amino acid 6-esters were synthesized by the same methods.


Examiners: Dr. D. Keglević, Dr. N. Pravdlić, and Prof. D. Sunko.


Dissertation deposited at the University Library, Zagreb and Institute »Ruder Bošković«, Zagreb.

(80 pages, 4 tables, 12 figures, 101 references, original in Croatian).

G. ROGLIC
1. Syntheses of Glucuronic Esters of Amino Acids

I. Roglic G.

II. "Ruder Bošković" Institute, Zagreb, Croatia, Yugoslavia

Accelerated active ester method
Amino acids, glucuronic esters with
Dicyclohexylcarbodi-imide method with imidazole
Glucuronic esters
Glucofuranuronic acid, methyl ester, 1-O-(acylaminoacyl)-2,3,5-tri-O-methyl-α- and β-D-
Glucopyranuronic acid, methyl ester, 1-O-(N-acyl-DL-alanyl)-2,3,5-tri-O-methyl-α- and β-D-
Glucopiranoside, 6-O-glycyl-β-D-
methyl
—, 2,3,4-tri-O-acetyl-6-O-(N-acetyl-glycyl)-β-D-
methyl
—, 2,3,4-tri-O-benzyl-6-O-(N-benzoxycarbonyl-aminoacyl)-β-
-D-
methyl
Sugar-amino acid linkage
Radiometric Investigation of Ca-Phosphates

N. Filipović-Vinčeković

Institute »Ruder Bošković«, 41000 Zagreb, Croatia, Yugoslavia

Radiometric procedures for fast determination of the solubility limits, precipitation kinetics, and precipitate equilibration of Ca-phosphates with the supernatant have been developed. The results of radiometric analysis show the formation of variously soluble Ca-phosphates. Solubility limits correspond to four morphological limits at the precipitation diagram established by Füredi and co-workers.

Analysis of the data on $^{45}$Ca and $^{32}$P radionuclide distribution in systems at 25°C show that the precipitates of Ca-phosphates pass through two steps: after formation of the metastable colloidal defectiveapatite acidic Ca-phosphate will be formed as a product corresponding to the second precipitation step. Depending on the initial conditions, OCP or DCP will be formed as a second product. By aging in the supernatant amorphous and unstable Ca-phosphates grow to the stable Ca-phosphate composition via Ostwald ripening and structural changes.

Examiners: Dr. R. Despotović, Dr. H. Füredi, and Prof. B. Težak

Oral examination: March 10, 1972

Thesis deposited at the Faculty of Science, University of Zagreb.

(128 pages, 21 table, 38 figures, 131 reference)
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<td>Precipitation</td>
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Radiometric Investigation of Stable AgI—I Sols

B. Subotić

"Ruder Bošković" Institute, 41000 Zagreb, Croatia, Yugoslavia

Heterogeneous exchange in the AgI—I system was investigated by means of the radioactive tracer technique. As a selected problem, the phenomenon of the acceleration of the exchange caused by the addition of coagulating electrolyte was examined. The results show strong dependence of the exchange acceleration on the concentration of coagulation electrolytes up to the critical coagulation concentration. The analysis of this phenomenon shows the influence of the coagulation electrolyte on the "methoric mass" of silver iodide, indicating that in silver iodide suspensions three fractions of colloid subsystems could be obtained: embryonal silver iodide, fraction of the metaphase mass, and methoric silver iodide. During the aging the embryos disappear by transforming into the solid phase, the silver iodide particles grow and the methoric mass disappears too turning into the solid phase.

Examiners: Dr. R. Despotović, Prof. M. Mirnik, Prof. R. Wolf
Oral examination: March 10, 1972

Thesis deposited at the Faculty of Science, University of Zagreb.

(163 pages, 32 figures, 2 tables, 106 references, original in Croatian)

R. DESPOTOVIC
<table>
<thead>
<tr>
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<tr>
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<td>Analysis, radiometric investigation of Silver Iodide, formation of sols, colloidal analysis of —, colloidal</td>
</tr>
<tr>
<td>II. Institute »Ruder Bošković«, 41000 Zagreb, Croatia, Yugoslavia</td>
<td>Analysis, radiometric investigation of Silver Iodide, formation of sols, colloidal analysis of —, colloidal</td>
</tr>
</tbody>
</table>
Numerical and Analytical Investigation of Complicated Molecular Integrals

A. Graovac

Institute "Ruder Bošković", 41000 Zagreb, Croatia, Yugoslavia

Two methods of evaluation of complicated molecular integrals over Slater-type orbitals are presented.

Three center nuclear-attraction integrals are calculated using the analytical method given by Bosanac and Randić which is derived using the Neumann expansion and the expansion of Legendre functions of first and second kinds. Well known $A_n$, $\tilde{A}_n$, and $B_n$ functions are appearing as basic quantities. The final formula involves double infinite summation. After some trial calculations the requirement of accuracy has been put to $\epsilon = 10^{-7}$. This leads to between three and at the most eleven terms in outer $l$-summation. In such a way we obtained absolute accuracies of $10^{-3}$ to $10^{-6}$. Numerical results are obtained for linear and nonlinear molecules with the limitation $m=0$. The different combinations of Slater-type orbitals from $(1s)$ to $(4s)$ orbitals are included and the corresponding coefficients $a_{n,l}$ are tabulated (for some cases $m \neq 0$ too).

The formula for the general integrals with $m \neq 0$ is also given.

Multicenter electron repulsion integrals were calculated using a numerical Fourier transform method based on a formulation first given by Bonham, Peacher, and Cox and developed by Harris and Monkhorst. Spherical expansion of plane waves was introduced and this enabled an insight into the behavior and the derivation of a method for accurate calculation of Fourier transforms of two-center charge distributions. This enabled the calculation of three-center exchange integrals. Using the free choice of the origin of transforms coplanar four-center integrals were calculated. In both cases only $(1s)$ orbitals were used.

The convergence properties of the method were discussed. Absolute accuracies of $10^{-3}$ to $10^{-4}$ were obtained. Integrals with diffuse and not too asymmetrical charge distributions were computed to four or five significant figures. When highly asymmetrical or compact charge distributions arise the choice of the origins of transforms was found to be very important. These conclusions are expected to hold for general $(ns)$ orbitals as well.

The formula for general non-planar four-center integrals is given too and some possible further applications are mentioned.

A part of this work was published in *Intern. J. Quantum Chem.* 7 (1973) 233.

*Examiners:* Dr. N. Trinajstić, Dr. E. Coffou and Dr. J. N. Herak


Thesis deposited at the University of Zagreb.

(85 pages, 13 tables, 60 references, original in Croatian)

A. GRAOVAC
<table>
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<td>Molecular integrals, Slater-type orbitals</td>
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<td>Multicenter electron repulsion integrals, (ns) orbitals, numerical Fourier-transform method</td>
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<tr>
<td>Three center, nuclear-attraction integrals, A_n, A_n and B_n functions</td>
</tr>
</tbody>
</table>
Characterization of the Negative Concentration Maximum of Silver Bromide by Macromolecules and by Change of Temperature

V. Crnički

Institute of Physical Chemistry, University of Zagreb, 41000 Zagreb, Croatia, Yugoslavia

The precipitation phenomena in the region of negative concentration maximum of silver bromide were investigated at 20 and 60 °C by the in statu nascendi method using a Zeiss tyndallimeter in connection with a Pulfrich photometer.

The influence of surface active agents triton T-X-305 and gelatin on the sol in the region of negative concentration maximum was also examined. With triton T-X-305 both flocculation and stabilization effects were observed while gelatin only stabilized the sols. All the effects were found to be dependent on the concentration of excess potassium bromide.

The temperature dependence of the complex solubility limit of negative silver bromide sol was also studied. By cooling the saturated solution from 90 to 20 °C silver bromide precipitated in form of larger crystals. When adding water or solutions of electrolytes or macromolecules to the cooled systems, sols were formed showing H. O. T. S. during their formation.

Examiners: Prof. B. Težak, Prof. R. Wolf, and Dr. H. Füredi-Milhofer


Thesis deposited at Faculty of Science, University of Zagreb.

(92 pages, 33 figures, 66 references, original in Croatian)
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<td>II. Institute of Physical Chemistry, University of Zagreb, 41000 Zagreb, Croatia, Yugoslavia</td>
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<tr>
<th>Flocculation, of AgBr sols</th>
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<tr>
<td>Silver bromide sol</td>
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<td>—, temperature effect on Stabilization of AgBr sols</td>
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<td>Surface active agents —, effects on AgBr sols</td>
</tr>
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</table>
The Role of Ionic Interactions in the Coagulation Process

N. Kallay

Institute of Physical Chemistry, University of Zagreb, 41000 Zagreb, Croatia, Yugoslavia

The influence of several electrolytes and electrolyte mixtures on the rate of coagulation of the negative silver iodide sol was examined. The methods proposed by Težak and by Reerink and Overbeek were used.

A linear relationship between the log of the electrolyte concentration and log of the rate constant of coagulation was found in the case of KNO₃, Mg(NO₃)₂, La(NO₃)₃.

The coagulation concentrations of electrolytes KNO₃, K₂SO₄, KOH (total concn. of K⁺ ions) was found to be the same but the coag. concn. of K₂PO₄ was greater. The coag. concns. of acids (total concn. of H⁺ ions) decrease in the following order: CH₃COOH, H₃PO₄, H₂SO₄, HNO₃ but the coag. activities of H⁺ ions were found to be practically the same. The results were explained in terms of ion pairing between counter and co-ions.

The observed antagonistic effects in the case of electrolyte pairs Mg(NO₃)₂-KNO₃ and Mg(NO₃)₂-HNO₃ were explained with general ionic interactions in the bulk of solution, and quantitatively interpreted using the Debye-Hückel theory. Constant coag. activity of Mg⁺ ions was found in spite of the increase of the KNO₃ and HNO₃ concentrations.

The observed antagonistic effects in the case of electrolyte pairs: Mg(NO₃)₂-K₂SO₄, Mg(NO₃)₂-H₂SO₄, Mg(NO₃)₂-H₃PO₄, Mg(NO₃)₂-N(CH₃)₂SO₄, La(NO₃)₃-K₂SO₄ were explained by ion pairing between counter- and co-ions. On the basis of experimental results the dissociation constants of ion pairs MgSO₄ and LaSO₄⁺ were calculated. The values were found to be in agreement with the literature results obtained by conventional methods.

The method for determination of ion-pair stability constants by measuring the rate of coagulation of lyophobic colloids was developed.

A part of this work was published in Croat. Chem. Acta 45 (1973) 169.

Examiners: Prof. B. Težak, Prof. R. Wolf, and Dr. Z. Pučar.


Thesis deposited at the Faculty of Science, University of Zagreb.

(70 pages, 4 tables, 16 figures, 29 references, original in Croatian)
MCC-54 (Univ. Zagreb)

1. The Role of Ionic Interactions in the Coagulation Process

I. Kallay N.
II. Institute of Physical Chemistry, University of Zagreb, 41000 Zagreb, Croatia, Yugoslavia

Activity of ions
- effect on coagulation rate
Coagulation
- in electrolyte mixtures
- in strong electrolytes
- in weak electrolytes
- rate of
Ion pairs
- determination of
- stability constants of
- MgSO₄
- LaSO₄⁺
Chelating Properties of Proline and Some Prolyl Peptides

B. Kužnar

Institute for Medical Research, Yugoslav Academy of Sciences and Arts, 41001 Zagreb, Croatia, Yugoslavia

Acid dissociation constants of proline, L-prolylglycine, and glycyl-L-proline were determined by a potentiometric titration method at 20°C in 0.37 mol dm⁻³ NaNO₃. The composition of the complexes formed by the above mentioned ligands with bivalent ions of nickel, copper, zinc, cadmium, and lead was also ascertained and their stability constants determined. The complexes of investigated dipeptides were found to be more stable than would be predicted on the ground of theoretical considerations. This could be explained by assuming an additional coordination site — presumably the peptide nitrogen — to be active in complex formation although not taking part in protonation equilibria. The copper(II)-prolylglycine system proved to be more involved than the others so that only rough estimates of the complex formation constants could be obtained.

The work was reported at the Third Yugoslav Congress of Pure and Applied Chemistry, Ljubljana 1972.

Examiners: Prof. O. A. Weber, Prof. B. Težak, and Dr. V. Katović.


Thesis deposited at the University Library, Zagreb, Faculty of Science, Univ. of Zagreb, and Institute for Medical Research, Yugoslav Academy of Sciences and Arts, Zagreb.

(71 pages, 6 tables, 9 figures, 46 references, original in Croatian).

B. KUZNAR
**MCC-55 (Univ. Zagreb)**

1. Chelating Properties of Proline and Some Prolyl Peptides

I. Kužnar, B.
II. Institute for Medical Research, Yugoslav Academy of Sciences and Arts, 41001 Zagreb, Croatia, Yugoslavia

<table>
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<th>Chelate Compound</th>
<th>Metal</th>
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<td>Chelate Compounds</td>
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<td>Glycyl-L-proline</td>
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<td>Lead(II)</td>
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<td>Nickel(II)</td>
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<td>Proline</td>
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<tr>
<td>Prolylglycine</td>
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<tr>
<td>Zinc(II)</td>
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</table>
Electrometric Determination of the Constitutive Ion Adsorption on the Silver Halides

S. Musić

Institute «Ruder Bošković», 41000 Zagreb, Croatia, Yugoslavia

The adsorption of I\textsuperscript– ions on negative AgI sols was determined potentiometrically using the Ag/Ag\textsubscript{2}S electrode for the measurement of I\textsuperscript– and Ag\textsuperscript{+} ion activities. For the fresh sols in statu nascendi the linear decrease of the adsorbed amount with pI (pAg) and the change of the molar adsorption capacity calculated by the formula \((\text{ads. I}) / (\text{AgI}) \times \Delta \text{pl})\) at pl = pAg = 8, were reproduced. Molar adsorption capacity decreases with the increase of the concentration of NaI and AgNO\textsubscript{3} solutions, with the age of the sols and decreases too in the critical region of the concentration of counter ions from maximal to an approximately ten times lower value. The concentrations of counter ions in which the capacity is decreased to 50\% of its maximal value depend on the valency of the counter ion and follow the linear formulation of the Schulze-Hardy rule. It was also demonstrated that the variation of the adsorbed amount of I\textsuperscript– ions on dried «isoelectric» AgI equals the change in the amount of counter ions within the limits of experimental error. The decrease of the molar adsorption capacity in the flocculation region was demonstrated for Triton X 305, Na-dodecyl sulfate, n-mirestlylamine nitrate, n-laurylamine nitrate.

Examiners: Prof. M. Mirnik, Dr. R. Despotović and Prof. R. H. Wolf.


Thesis deposited at the University of Zagreb.

(58 pages, 15 figures, 55 references, original in Croatian)
MCC-56 (Univ. Zagreb)

1. Electrometric Determination of the Constitutive Ion Adsorption on the Silver Halides

I. Musić S.
II. Institute »Ruder Bošković«, 41001 Zagreb, Croatia, Yugoslavia

Adsorption capacity
AgI suspension, aging of
Potentiometry, determination
of adsorption capacity by
Schulze-Hardy rule
Surfactants,
influence on adsorption capacity
Investigation of the Process of Heterogeneous Exchange in the Systems AgI—I/Fluorescein and AgI—I/tetrachloro-tetraiodo-fluorescein

Z. Selir

Institute «Ruder Bošković», 41000 Zagreb, Croatia, Yugoslavia

The purpose of this work was to establish whether it is possible to apply consequently the Trauber principle to the organic molecules when their molecular mass increases by introducing small and heavy inorganic substituents. Sodium fluoresceinate (FLN) has been chosen as a model for the organic substance and sodium tetrachloro-tetraiodo-fluorescienate (BRB) has been used as a derivative Silver iodide sol, prepared in statu nascendi has been taken as the colloid system. General conditions were as follows: 0.01 M NaI, 0.01 M AgI, FLN or BRB from $1 \times 10^{-6}$ to $3 \times 10^{-3}$ M.

The experiments were carried out using various methods: tensometry, potentiometry, conductometry, turbidimetry, ultramicroscopic electrophoresis, X-ray diffractometry, microphotography, radiometric determination of the adsorption capacity and radiometric following of the process of heterogeneous exchange.

The results show that FLN and BRB behave differently under the same conditions of investigation: in relation to FLN, BRB behaves as an organic molecule with a large number of carbon atoms. Although these two substances have the same carbon skeleton, they have different inorganic substituents. From the analysis of the cited experiments and from the process of heterogeneous exchange it was concluded that the Trauber rule can also be extended to the effects caused by the increase of the mass of the organic molecule by introduction of heavier inorganic substituents.

Examiners: Dr. R. Despotović, Prof. M. Mirnik and Prof. R. H. Wolf.

Oral examination: December 22, 1972

Thesis deposited at the University of Zagreb.

(82 pages, 2 tables, 23 figures, 60 references, original in Croatian)

R. DESPOTOVIC
MCC-57 (Univ. Zagreb)

1. Investigation of the Process of Heterogeneous Exchange in the Systems AgI—I/Fluorescein and AgI—I/ Tetrachloro-tetraiodo-fluorescein

I. Selir Z.
II. Institute »Ruder Bošković«, 41001 Zagreb, Croatia, Yugoslavia

Exchange, heterogeneous
I
Fluorescein
—, tetrachloro-tetraiodo
Silver iodide sol
autodiffusion
recrystallization
Ostwald ripening
Traube rule
Characterization of the Precipitation System of Silver Chloride in the Solutions of Some Electrolytes and Macromolecules

N. Stubićar

Institute of Physical Chemistry, University of Zagreb, 41000 Zagreb, Croatia, Yugoslavia

The precipitation of silver chloride was investigated in the presence of nonionic surface-active agents of the OPE-series (Triton X-305), amphoteric polyelectrolyte gelatin (isoelectric point at pH = 4.7) and some electrolytes as: KNO₃, Ba(NO₃)₂, La(NO₃)₃. The concn. range between 10⁻⁴ and 10⁻¹ mol dm⁻³ AgCl was examined.

The precipitation was followed by tyndallometric measurements and the sign of the particle charge was confirmed by microscopic electrophoresis. The effect of added substances upon the shape and size of AgCl crystallites formed by cooling of supersaturated solns was also investigated by light and electron microscopy.

Stabilization and flocculation effects of triton and gelatin were obtained on both positively and negatively charged silver chloride sols in statu nascendi at 20°C. Flocculation has been less expressed on negatively charged sols, which are more stable than the positively charged sols.

AgCl crystallites of the approximately equal shape and size were prepared by cooling the complex solns from 90°C to 20°C in the presence of triton or gelatin in greater concn. than c.c.c. or in the presence of electrolyte in greater concn than c.c.c. At their flocculating or coagulating concns, however, crystallites of various size and shape were obtained.

In dependence of the concentrational relationships of AgCl and of the added substances, studied systems show various colloid and crystalline characteristics.

Examiners: Prof. B. Težak, Prof. R. Wolf and Dr. R. Despotović.


Thesis deposited at the Faculty of Science, University of Zagreb.

(104 pages, 43 figures, 53 references, original in Croatian)

N. STUBICAR
MCC-58 (Univ. Zagreb)

1. Characterization of the Precipitation System of Silver Chloride in the Solutions of Some Electrolytes and Macromolecules

I. Stubičar N.

II. Institute of Physical Chemistry, University of Zagreb, 41000 Zagreb, Croatia, Yugoslavia

Flocculation by nonionic surface-active agents (Triton X-305)
by amphoteric polyelectrolyte gelatin
Monodisperse sol(s) of silver chloride
Silver chloride sol(s)
precipitation of flocculation of crystallization of
Stabilization by gelatin
by nonionic surface-active agents (Triton X-305)
Adsorption of Tri-n-butyl Phosphate from Aqueous Solutions on the Mercury Electrode and its Influence on the Electrode Processes of some Metal Ions

D. Krznarić

Center for Marine Research, Institute »Ruder Bošković«, 41000 Zagreb, Croatia, Yugoslavia

The adsorption of tri-n-butyl phosphate (TBP) on the mercury electrodes from aqueous solutions, and its influence on the electrode processes of Tl(I), Cu(II), Cd(II), Pb(II), In(III), and U(VI) was investigated by means of d.c. polarography, Kalousek commutator, and double potential-step chronocoulometry.

Four different methods for the determination of TBP concentration in aqueous solutions, are proposed. Two of the methods employ Kalousek commutator, while the other two consist of different modes of application of double potential-step chronocoulometry. These methods enable the determination of TBP concentration in aqueous solution from $5 \times 10^{-6}$ M up to $2 \times 10^{-3}$ M.

The investigated metal ions can be divided into four different groups according to their electrode processes in the presence of TBP. One type of behaviour is represented by the Tl(I) ion, the next one by Cu(II), Cd(II), and Pb(II) ions, the third by In(III), and the fourth one by the U(VI) ion.

The presence of TBP does not influence the electrode processes of Tl(I), while the electrode processes of In(III), in chloride medium, are almost completely inhibited by the layer of TBP on the electrode. From the current-time curves of Pb(II), Cd(II), and Cu(II) it is evident that the inhibition of the electrode processes, on the covered surface, increases with the acidity of the solution and also with the increase of the bulk concentration of TBP. Contrary to this, the change of the concentration of TBP does not affect the reduction process of the uranyl ion. This can be attributed to the fact that the uranyl ion is not reduced to the amalgam like the other investigated metal ions. It is therefore supposed that the possible effect of the formed amalgam should be considered.

No adsorption of the reactants was found by chronocoulometric measurements for the electrode processes of the mentioned metal ions in the presence of TBP. It was concluded therefore that the complex formation between metal ions and TBP does not occur on the electrode surface prior to the electrode process. The adsorbed TBP most probably affects chemical reactions, such as dehydration, which could be involved in the electrochemical processes of Cd(II), Pb(II), Cu(II), and In(III) ions.

Part of this work was reported at the 3rd Yugoslav Congress on Pure and Applied Chemistry, Ljubljana 1972. A part of the thesis was published in: J. Electroanal. Chem. 44 (1973) 401–410.

Examiners: Dr. M. Branica, Prof. I. Filipović, and Prof. B. Težak.


Thesis deposited at the Institute »Ruder Bošković«, Zagreb, and the University Library, Zagreb.

(115 pages, 32 figures, 81 references, original in Croatian)

D. KRZNARIC
1. Adsorption of Tri-n-Butyl Phosphate from Aqueous Solutions on Mercury Electrodes and Its Influence on the Electrode Processes of some Metal Ions

I. Krznaric D.
II. Center for Marine Research, Institute « Ruder Bošković», 41000 Zagreb, Croatia, Yugoslavia

Adsorption of tri-n-butyl phosphate on mercury electrodes. Metal ions, influence of the adsorption of tri-n-butyl phosphate on the electrode processes of tri-n-butyl phosphate, adsorption of, on mercury electrodes from aqueous solutions,
Graph Theory and Molecular Orbitals

I. Gutman

Institute »Ruder Bošković«, 41000 Zagreb, Croatia, Yugoslavia

Graph theory (GT) has been proved to be a suitable mathematical technique for molecular orbital (MO) studies of conjugated hydrocarbons. Necessary notions of GT including Sachs theorem are presented. The commutation relations between the Hückel Hamiltonian and the graph adjacency matrix (A) is discussed. It is shown that the MO's and MO energies are identical with the eigenvectors and eigenvalues of A, respectively.

The pairing theorem is analysed from several points of view. It is shown that the number of zero eigenvalues (NZE) of A determines the stability of conjugated hydrocarbons. Nine new theorems for calculating and/or estimating the NZE’s are presented.

The total π-electron energy (E) is shown to be a function of A. It is found that the Hückel (4m + 2)-rule can be generalized to all conjugated hydrocarbons and a new »loop rule« has been derived. Using the loop rule approximate expressions for E and general rules governing the dependence of E on molecular structure are obtained.


Examiners: Dr. N. Trinajstić, Dr. D. Cvetković, and Dr. Z. Maksić.


Thesis deposited at the University of Zagreb and the Institute »Ruder Bošković«, Zagreb.

(47 pages, 37 references, original in Croatian)
MCC-60 (Univ. Zagreb)

1. Graph Theory and Molecular Orbitals
   I. Gutman I.
   II. Institute «Ruder Bošković», 41000 Zagreb, Croatia, Yugoslavia

Conjugated hydrocarbons
Graph theory
Hückel
—, rule
—, theory
Molecular orbitals
Topology
Secondary Deuterium Isotope Effects in Solvolysis of Cyclopentyl p-Bromobenzenesulfonate. Stereochemistry of E1 and SN1 Reactions

V. Sendijarević

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Secondary α- and β-isotope effects in solvolysis of cyclopentyl-1-d, cis-cyclopentyl-2-d, trans-cyclopentyl-2-d, and cyclopentyl-2,2,5,5-d4 broxylates were measured in different ethanol—water (E-W) and trifluoroethanol—water (TFE) mixtures. The magnitude of the effects indicates that in the E-W mixtures the products are derived by rate determining substitution and elimination on the reversibly formed intimate ion pair. However, the change to TFE—W mixtures causes a change in mechanism; in these solvents the formation of the solvent separated ion pair is rate determining and the products are formed in fast subsequent attack on this intermediate. Consistent with this interpretation of the isotope effects, the elimination in E—W mixtures was found to be stereospecifically trans, while in TFE—W mixtures it is nonstereospecific. It was also determined that the configuration of the cyclopentanol formed in both types of solvent was inverted in comparison to the starting material. A detailed analysis provides an estimation of the isotope effects in each of the individual steps in the reaction.

A part of this work was published in J. Amer. Chem. Soc. 95 (1973) 7722.

Examiners: Dr. K. Humski, Dr. S. Borčić and Dr. A. Deljac.


Thesis deposited at the University of Zagreb.

(51 pages, 10 figures, 20 tables, 74 references, original in Croatian)
1. Secondary Deuterium Isotope Effects in Solvolysis of Cyclopentyl p-Bromobenzenesulfonate. Stereochemistry of $E1$ and $S_{N1}$ Reactions

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MCC-61 (Univ. Zagreb)

Cyclopentyl derivatives, solvolysis of Isotope effects, deuterium, secondary Solvolysis Stereochemistry, of $E1$ and $S_{N1}$ reactions
Solvolysis of Menthyl and Neomenthyl Tosylates. Conformation and Secondary Deuterium Isotope Effects

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Transition states geometries in solvolyses of menthyl and neomenthyl tosylates were studied by means of secondary α- and β-deuterium isotope effects and product analyses.

α-Effects of both menthyl and neomentyl tosylates are »normal« indicating that in the transition state(s) there is almost no covalent bonding between the α-carbon and either the leaving group or the nucleophile.

The value of β-d₃ isotope effect of neomenthyl tosylate, however, is approximately twice as high as that of mentyl tosylate. The neomenthyl tosylate has two hydrogen atoms antiparallel to the leaving group, therefore ideally suited for participation. The only substitution products found in solvolysis of neomentyl tosylate were rearranged alcohol, 1-methyl-4-isopropyl cyclohexane-4-ol, and some amount of alcohol with retained configuration at the reaction center, neomenthol. In olefinic products Δ'-menthene predominates although exocyclic Δ¹α-menthene was also formed. Such products composition indicate that a hydrogen bridged cation exists as an intermediate in solvolysis of neomenthyl tosylate. This is in accord with the observed high value of β-deuterium isotope effect.

Menthyl tosylate has no β-hydrogens antiparallel to the leaving group. In a twisted transition state, one of β-hydrogen atoms could assume the antiparallel arrangement favourable for participation. However, the observed β-d₃-isotope effect is quite normal indicating that menthyl tosylate solvolyzes via a rigid chair-like transition state. The main substitution product in solvolysis (besides ethers) is menthol. This could also be explained by the chair-like transition state. In a twisted, half-chair conformation of transition state the product with predominately inverted configuration at the reaction center would be formed.

It may be concluded that β-deuterium isotope effects in combination with product analysis are an efficient tool for conformational analyses of transition states in solvolyses of cyclohexyl derivatives. Both neomenthyl and menthyl tosylates solvolyze via chair-like transition states but only the solvolysis of neomenthyl tosylate includes the participation of tertiary β-hydrogen.

Dissubstituted cyclohexyl derivatives with equatorial leaving group appear to solvolzye via a rigid transition state only if a voluminous alkyl substituent is in the β-position to the leaving group while another alkyl group is substituted at the position 3 or 4.

Examiners: Dr. D. E. Sunko, Dr. Z. Majerski, and Dr. T. Cvitaš


Thesis deposited at the University of Zagreb.

(101 pages, 20 figures, 22 tables, 92 references, original in Croatian)

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1. Solvolysis of Menthyl and Neomenthyl Tosylates. Conformation and Secondary Deuterium Isotope Effects

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Conformation, of transition states
Cyclohexyl derivatives,
solvolysis of
Isotope effects, deuterium,
secondary Participation, neighbouring
hydrogen Solvolysis
Glucoyl Esters of Amino Acids and Dipeptides

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Fully protected o-glucopyranosyl esters of amino acids and dipeptides were synthesized via two routes involving direct participation of imidazole in the 1-ester linkage formation: (a) the »accelerated active-ester« method, and (b) the imidazol-promoted dicyclohexylcarbodiimide condensation. The amino function in the aglycon group was protected by the tert-butylxycarbonyl or benzoxycarbonyl group, and the hydroxyl functions of the sugar moiety were fully benzylated or acetylated. The products were obtained in good yields as anomeric mixtures which were sep.d. and fully characterized.

Catalytic hydrogenation of the tetrabenzyl ethers of 1-O-tert-butylxycarbonylaminocarbamyl-β-D-glucopyranoses afforded the corresponding 1-O-acrylamidocarbamyl-β-D-glucopyranoses; their structures were confirmed by conversion into the peracetylated derivs. Debenzylation of the α-remomers resulted in 1→2 O-acyl migration; the rearrangement product of 1-O-(tert-butylxycarbonyl-L-alanyl)-β-D-glucopyranose was identified by conversion into the corresponding 1,3,4,6-tetra-O-acetyl deriv, which was also synthesized by definitive methods. Deprotection of the tert-butylxycarbonyl group with trifluoroacetic acid afforded 1-O-glycyl-β-D-glucopyranose in the form of crystalline trifluoroacetate.

Catalytic hydrogenation of the fully benzylated 1-O-[N-benzyloxycarbamyl-dipeptidyl]-β-D-glucopyranoses (dipeptidyl=glycylglycyl, L-alanyl-glycyl) gave the corresponding glucosyl esters as the crystalline monooxalate salts. Their structures were confirmed by conversion into the corresponding N-acetyl derivatives.

Part of this thesis are published in Carbohydr. Res. 22 (1972) 245; ibid. 29 (1973) 25.

Examiners: Dr. D. Keglević, Prof. D. Sunko, and Dr. N. Pravdić.


Thesis deposited at the University of Zagreb and the Institute »Ruder Bošković«, Zagreb.

(88 pages, 12 figures, 5 tables, 83 references, original in Croatian)

S. VALENTEKOVIC
1. Glucosyl Esters of Amino Acids and Dipeptides

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II. Tracer Laboratory, Institute »Ruder Bošković«, 41000 Zagreb, Croatia, Yugoslavia

Accelerated active ester method
Amino acids, glucosyl esters with Dicyclohexylcarbodi-imide method
Dipeptides, glucosyl esters with Glucosyl esters
Imidazole
Sugar-amino acid ester linkage
Catalytic Hydrogenation of 2,2'-Bisoxalines

G. Strohal
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N,N'-Bis(α-hydroxyalkyl)ethylenediamines can be obtained by hydrogenolysis of 2,2'-bisoxazolines with Pt/Rh or Adams catalyst. This method was used for the preparation of well known tuberculostatics (+)-N,N'-bis (1-hydroxymethylpropyl)-ethylenediamine from (-)-4,4'-diethyl-2,2'-bisoxazoline in almost quantitative yield.

The best reaction conditions were found to be Pt/Rh catalyst, methanol, ethanol or ethylacetate as a solvent, 50 atm hydrogen pressure and room temperature.

A series of unknown 2,2'-bisoxazolines was prepared but only 2,2'-bisoxazolines without an aliphatic or aromatic group in the 2,2'-positions were successfully hydrogenolized.

Examiners: Dr. K. Jakopčić, Dr. I. Butula, and Prof. I. Lovreček


Thesis deposited at the University of Zagreb.

(76 pages, 22 figures, 3 tables, 38 references, original in Croatian)

G. STROHAL
MCC-64 (Univ. Zagreb)

1. Catalytic Hydrogenation of 2,2'-Bisoxalines
   I. Strohal G.
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(±)-N,N'-Bis(1-hydroxymethylpropyl)-ethylenediamine, preparation of 2,2'-Bisoxazolines, hydrogenolysis of Tuberculostatics
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Zavod za farmakologiju, Farmaceutsko-biokemijski fakultet, Zagreb and Zavod za organsku kemiju, Kemijsko-tehnološki fakultet, Split
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Institut za organsku kemiju i biokemiju Sveučilišta u Zagrebu and Institut za farmakologiju i tоксикологију Medicinskog fakulteta, Sarajevo
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M. Fleš
Imunološki institut, Zagreb
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Zavod za kemiju i biokemiju, Medicinski fakultet, Rijeka i Zavod za kemiju i biokemiju, Medicinski fakultet Zagreba, Sveučilište u Zagrebu
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L. Gutman and N. Trinajstić
Institute «Rudjer Bošković», P. O. Box 1016, 41001 Zagreb, Croatia, Yugoslavia

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L. Klasinc and H. Guesten
Institut für Radiochemie, Kernforschungszentrum Karlsruhe, Karlsruhe, Germany

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L. Klasinc, J. V. Knog, H. J. Meiners und W. Zeihl
Institut für Physikalische Chemie der Universität Ulm

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A. Kornhauser and M. A. Pathak
Harvard Medical School, Department of Dermatology at the Massachusetts General Hospital, Boston, Massachusetts 02114

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M. Movrin
Zavod za farmaceutsku kemiju, Farmaceutsko-blokemijski fakultet 
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Department of Chemistry, Faculty of Science and Mathematics, University of Zagreb, Zagreb, Croatia, Yugoslavia and Laboratory of Physical Chemistry, Institute »Boris Kidrič«, Belgrade, Serbia, Yugoslavia

Hybridization in Fused Strained Rings by the Maximum Overlap Method. II. Benzocyclobutene and Benzocyclopropene

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Influence of Some Compounds Similar to L-Asparagine on the Growth of Malignant Tumours in the Mouse

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P. Strohal, I. Bačić, B. Katić, and Ž. Selec
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Institute Ruder Bošković, Zagreb, Yugoslavia and College William and Mary, Williamsburg, Virginia 23185, U. S. A.

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Institute of Organic Chemistry and Biochemistry of the University, Strassmayerov trg 14, YU-41000 Zagreb

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J. E. Bloor and Z. B. Maksić
Chemistry Department, The University of Tennessee, Knoxville, Tennessee 37916, U. S. A. and Institute »Ruder Bošković«, 41001 Zagreb, Croatia, Yugoslavia
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N. Bodor, M. J. S. Dewar, and Z. B. Maksić
Department of Chemistry, University of Texas at Austin, Austin, Texas 78712
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Lj. Bokić and I. Filipović
Institute of Inorganic and Analytical Chemistry, University of Zagreb, and Laboratory of Inorganic Chemistry, Faculty of Technology, Zagreb (Yugoslavia)
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J. Chevalet and V. Žutić
Center for Marine Research, Ruder Bošković Institute, P. O. Box 1016, 41001 Zagreb, Croatia (Yugoslavia)
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D. Cvetković, I. Gutman, and N. Trinajstić
Faculty of Electrical Engineering, University of Belgrade, 11001, Belgrade, Serbia, Yugoslavia and Institute Ruder Bošković, P. O. Box 1016, 41001 Zagreb, Croatia, Yugoslavia
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L. Dubić, S. Szechter, and S. Shrinivasan
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Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia
Radical Pairs in Irradia ted Single Crystals of 1-methyl U racil

BCC-1222
P. McFadyen and E. Matijević
Institute of Colloid and Surface Science and Department of Chemistry,
Clarkson College of Technology, Potsdam, New York 13676
Precipitation and Characterization of Colloidal Copper Hydrous
Oxide Sol s

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P. McFadyen and E. Matijević
Institute of Colloid and Surface Science and Department of Chemistry,
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Institute »Ruder Bošković«, 41001 Zagreb, Croatia, Yugoslavia
Secondary Dueterium Isotope Effects in the Solvolysis of
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BCC-1225
A. Graovac, I. Gutman, M. Randić, and
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Institute »Ruder Bošković«, 41001 Zagreb, Croatia, Yugoslavia and
Department of Chemistry, Harvard University, Cambridge, Massachusetts
02138
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D. Grđenić and M. Sikirica
Laboratory of General and Inorganic Chemistry, Faculty of Science, University of Zagreb, 41001 Zagreb, Croatia, Yugoslavia
Crystal Structure of Mercury (II) Hydroxide Fluoride

BCC-1227
H. Guesten, L. Klasinc, and D. Stefanović
Institut für Radiochemie Kernforschungszentrum Karlsruhe, Karlsruhe, Germany
Electron Impact Induced Fragmentation of Substituted 4-Styryl Quinolines

BCC-1228
I. Gutman and N. Trinajstić
Institute »Ruder Bošković«, 41001 Zagreb, Croatia, Yugoslavia
Graph Theory and Molecular Orbitals. The Loop Rule

BCC-1229
M. J. Herak and V. Jagodić
Institute »Ruder Bošković«, 41001 Zagreb, Croatia, Yugoslavia
Distribution and Dimerization of Organophosphorus Extractants and Their Extraction Efficiency in Different Solvents

BCC-1230
M. J. Herak, M. Janko and B. Tamhina
Laboratory for Analytical Chemistry, Faculty of Science and Institute of Inorganic and Analytical Chemistry, University of Zagreb, Yugoslavia
Extraction, Complex Formation and Spectrophotometric Determination of Iron(III) with 2-Carbethoxy-5-hydroxy-1-(4-tolyl)-4-pyridone

BCC-1231
M. J. Herak, B. Tamhina and K. Jakopčić
Institute of Inorganic and Analytical Chemistry, University of Zagreb and Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia
Extraction and Separation of Gallium(III) from Zinc(II) by 2-Carbethoxy-5-hydroxy-1-(4-tolyl)-4-pyridone

BCC-1232
M. Hercet and R. Weiss
Institut Chimie, Université Louis Pasteur, BP 296/R8, 67008 Strasbourg Cedex, France
Structure Cristalline et Moléculaire du 1,7,10,16-Tétraoxaa-4,13-diazacyclooctadécane-dichloro-cuivre(II)

BCC-1233
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The Crystal Structure of Mercury(I) Orthoarsenate

BCC-1235
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Tracer Laboratory, Institute »Ruder Bošković«, Zagreb (Yugoslavia)
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BCC-1236
L. Klaić, N. Trinajstić and E. Pop
Institute »Ruder Bošković«, P. O. Box 1016, 41001 Zagreb, Croatia, Yugoslavia
Theoretical Study of Isomeric Thiienylfurans

BCC-1237
K. Kovačević and M. Proštenik
Zavod za kemiju i biokemiju Medicinskog fakulteta i Institut za organsku kemiju i biokemiju Sveučilišta u Zagrebu
Chromatographic Identification of Long-Chain 2,3-Dihydroxy Fatty Acids

BCC-1238
B. Kojić-Prodić, R. Liminga and S. Šćavnićar
Institute »Ruder Bošković«, 41001 Zagreb, Box 1016, Yugoslavia
The Crystal Structure of Caesium Oxobisoxalatobisaquoniobate(V) Dihydrate, Cs[NbO(C2O4)2(H2O)2] • 2H2O

BCC-1239
K. Kovac and Z. B. Maksić
Institute »Ruder Bošković«, 41001 Zagreb, Croatia, Yugoslavia
Calculation of 1J(13C—29Si) Spin-Spin Coupling Constants by the Maximum Overlap Approximation Method

BCC-1240
D. Krbzanić, B. Čosović and M. Brnić
Center for Marine Research, »Ruder Bošković«, Zagreb, Croatia (Yugoslavia)
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S. Kukolja and S. R. Lammert
The Lilly Research Laboratories, Eli Lilly and Comp., Indianapolis, Indiana 46206 (USA)
Synthese von Desacetoxycephalosporin-S-oxiden aus Penicillin-S-
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B. Kunst and B. Floreani
Institute of Physical Chemistry, Technology Department, University of Zagreb, Zagreb, Yugoslavia and »Pliva«, Pharmaceutical and Chemical Works, Zagreb (Yugoslavia)
On the Preparation of Highly Permeable Cellulose Acetate Ultrafiltration Membranes

BCC-1243
B. Kunst, B. Lovreček and O. Hergula
Institute of Electrochemistry and Electrochemical Technology, Faculty of Technology, University of Zagreb, 41000 Zagreb, Savska c. 10/1 (Yugoslavia)
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A. Lutkić and V. Fišter
Zavod za fiziologiju, Medicinski fakultet, Sveučilište u Zagrebu
Glycogen Formation and Structure in the Rat Liver in Different Metabolic States

BCC-1245
V. Magnus, S. Iskrić and S. Kveder
»Ruder Bošković«, P. O. Box 1016, YU-41001 Zagreb, Yugoslavia
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Z. B. Maksić and J. E. Bloom
Institute »Ruder Bošković«, 41000 Zagreb, Yugoslavia and Department of Chemistry, The University of Tennessee, Knoxville, Tennessee 37916
An Additivity Equation for Calculating Second Moments of the Electronic Charge Distribution

BCC-1247
Z. B. Maksić, Z. Meić and K. Kovačević
Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia
MOA Calculations of CH Stretching Frequencies and Dissociation Energies in Hydrocarbons

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Z. B. Maksić and M. Randić
Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia
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E. Matijević, A. Bell, R. Brace and P. McFadyen
Institute of Colloid and Surface Science and Department of Chemistry, Clarkson College of Technology, Potsdam, New York 13696
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S. Mesarić and E. A. M. F. Dahmen
Department of Chemical Technology, Twente University of Technology, Enschede (The Netherlands) and Institute »Ruder Bošković«, Zagreb, Yugoslavia

Ion-Selective Carbon-Paste Electrodes for Halides and Silver(I) Ions

BCC-1251
M. Movrin and D. Majšinger
Zavod za farmaceutsku kemiju, Farmaceutsko-biokemijski fakultet Sveučilišta u Zagrebu

5,6-Quinolinequinones as Potential Chemotherapeutics

BCC-1252
D. M. Novak-Adamić, B. Ćosović, H. Bilinski and M. Branica
Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia

Precipitation and Hydrolysis of Metallic Ions-V. Nickel(II) in Aqueous Solutions

BCC-1253
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Kinetics and Mechanism of Replacement of Nitrosobenzene in the Pentacyanid(nitrosobenzene) Ferrate(II) Ion by Cyanide Ion

BCC-1254
I. Perina, N. Bregant and K. Balenović
Institut za organsku kemiju i biokemiju Sveučilišta u Zagrebu

Oxidations with Selenoxides. IV. Reaction of O-Dihydric Phenols with Diphenyl Selenoxide and Diphenylselenium Dichloride

BCC-1255
I. Perina, N. Bregant and K. Balenović
Institut za organsku kemiju i biokemiju Sveučilišta u Zagrebu

Oxidations with Selenoxides. V. Reaction with L-Ascorbic Acid with Diphenyl Selenoxide

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M. Peteš and S. Bruckenstein
Chemistry Department, State University of New York at Buffalo, Buffalo, N.Y. 14214 (U.S.A.)

An Isotopic Labeling Investigation of the Mechanism of the Electrooxidation of Hydrazine at Platinum
BCC-1257
J. Petričić, L. Holik, N. Drnovšek-Hlavkai L. Mijalić
Zavod za ispitivanje i kontrolu lijekova SRH, Zagreb, M. Pijade 180
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I. Piljac, B. Grabarić and I. Filipović
Laboratory of Inorganic Chemistry, Faculty of Technology and Institute
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Improved Technique for Determination of Stability Constants
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BCC-1259
B. Pokrić and Z. Pučar
Laboratory for Electrophoresis, Institute »Ruder Bošković«, Zagreb,
Yugoslavia
Electrophoretic and Tyndallometric Studies on the Hydrolysis
of Lead(II) in Aqueous Solutions

BCC-1260
B. Pokrić and Z. Pučar
Laboratory for Electrophoresis, Institute »Ruder Bošković«, Zagreb,
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BCC-1261
M. Popović und M. Proštenik
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B. Rasporn and M. Branića
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J. Šipalo-Žuljević and R. H. H. Wolf
»Ruder Bošković« Institute, Zagreb, Croatia, Yugoslavia
Sorption of Lanthanum(III), Cobalt(II) and Iodide Ions at Trace Concentration on Ferric Hydroxide

BCC-1267
V. Sunjić, F. Kajfež and D. Kolbah
CRC, Compagnia di Ricerca Chimica, Chiasso, Switzerland, and Institute of Organic Chemistry and Biochemistry, University of Zagreb, Yugoslavia
Stereochemistry of the Palonovski Rearrangement 1,4-Benzodiazepines-N-oxides; 2,3-Sigmatropic Shift; Ammonium Ylides

BCC-1268
B. Tamhina, M. Herak and K. Jakopčić
Institute of Organic and Analytical Chemistry, University of Zagreb and Institute »Ruder Bošković«, Zagreb, Croatia (Yugoslavia)
The Extraction and Separation of Gallium from Zinc by Derivatives of Pyridone

BCC-1269
J. Tomašić and D. Keglević
Tracer Laboratory, Institute »Ruder Bošković«, 41001 Zagreb, Yugoslavia
The Kinetics of Hydrolysis of Synthetic Glucuronic Esters and Glucuronic Ethers by Bovine Liver and Escherichia coli β-Glucuronidase

BCC-1270
N. Vuletić and C. Djordjević
Institute »Ruder Bošković«, Zagreb, Yugoslavia and College of William and Mary, Williamsburg, Virginia 23185, U.S.A.
Oxodiperoxovanadate(V) Complexes with Bidentate Ligands
Co-ordination Complexes of Niobium and Tantalum, Part XIV. Alkoxo-(2,2'-bipyridine)trichloroniobium(IV) Complexes


Interaction between Hexanocyanoferrate(II) Ion and Mercury(II) and Silver(I) Ions