

DCC-42 (Univ. Zagreb)

Croat. Chem. Acta

CCACAA 46 (4) B1—B2 (1974)

**The Sulphur-34 and Deuterium Isotope Effects in the  
Decomposition of Sulphones**

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Reaction between phenyl sulphone and sulphur was studied in the melt, at various temperatures, and SO<sub>2</sub> production was measured.

The kinetics in nitrogen atmosphere was studied at 243, 262, 288, and 297 °C and the corresponding first order rate constants,  $k \times 10^6 \text{ s}^{-1}$ , were found to be  $5.21 \pm 0.12$ ,  $19.2 \pm 0.3$ ,  $120 \pm 1.00$ ,  $209 \pm 9.00$ , respectively (uncertainties are standard deviations).

Using the technique of least squares the energy of activation was found to be  $41 \pm 1.00 \text{ kcal mol}^{-1}$ , the frequency factor  $1.00 \times 10^{12} \text{ s}^{-1}$ , and entropy of activation  $-7.00 \text{ cal mol}^{-1} \text{ K}^{-1}$ .

The sulphur-34 isotope effect was found to be 0.43% at 243 °C. The value of the sulphur-34 isotope effect was corrected, because of the reduction process, and it amounted to 0.87%. The maximum sulphur-34 isotope effect for decomposition of the hypothetical C-S molecule was calculated to be 1.07% at the same temperature. The experimental value of the sulphur-34 isotope effect indicated appreciable C-S bond weakening in the transition state, and suggested the dissociation as the rate determining step.

The decomposition of cyclic sulphones was also studied at various temperatures, and SO<sub>2</sub> produced in the reaction was measured.

The kinetic data were used to determine the energy of activation, frequency factor and entropy of activation as  $33.2 \text{ kcal mol}^{-1}$ ,  $7.10 \times 10^{14} \text{ s}^{-1}$ , and  $7.00 \text{ cal mol}^{-1} \text{ K}^{-1}$ , respectively, which is in good agreement with literature data.

The sulphur-34 isotope effect was determined in the decomposition of 2,5-dihydrothiophene-1,1-dioxide in the melt and was found to be 0.97% at 99.5 °C.

The  $\alpha$ -deuterium isotope effects were measured in the decomposition of 2,5-dihydrothiophene-2,2,5,5-d<sub>4</sub>-1,1-dioxide at 120 °C and 2,4-dimethyl-2,5-dihydrothiophene-5,5-d<sub>2</sub>-1,1-dioxide at 105 °C in the melt and they amounted to 9.4 and 5.4%.

The value of  $\alpha$ -deuterium isotope effects and the value of sulphur-34 isotope effects indicates the concerted mechanism of this reaction, which is one example of a retro Diels-Alder reaction, as it was also predicted by the Woodward-Hoffman rules.

The thesis was partly published in: *J. Org. Chem.* 36 (1971) 3845 and *J. Org. Chem.* 37 (1972) 1745.

Examiners: Prof. S. Ašperger, Prof. D. Sunko, and Dr. N. Trinajstić.

Oral examination: July 6, 1971.

Degree conferred: October 28, 1971.

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(144 pages, 22 tables, 6 figures, 173 references, original in Croatian).

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*DCC-42 (Univ. Zagreb)*

1. The Sulphur-34 and Deuterium  
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of Sulphones

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Decomposition of sulphones  
Isotope effects,

—, deuterium  
—, sulphur-34

Sulphones, decomposition of

DCC-43 (Univ. Zagreb)

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**Investigation of Topological Properties of Conjugated Hydrocarbons**

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Using the mathematical apparatus of graph theory several properties of conjugated hydrocarbons were analyzed.

Upper and lower bounds for the total  $\pi$ -electron energy were determined. The structure of the molecular graph is related to the energy by applying the loop rule. Several approximate expressions for energy are obtained.

The relation between the number of Kekulé structures and the determinant and permanent of the adjacency matrix is found both for alternant and non-alternant hydrocarbons.

The class of graphs representing benzenoid hydrocarbons is rigorously defined and a number of theorems is proved for this class. It is shown that the Ruedenberg and Pauling bond orders are identical, a formula of Heilbronner is improved and a relation between the coefficients of the non-bonding MO and VB spin density is found. Strict limits of validity of all these results are given.

Rules governing the  $\pi$ -electron charge distribution in non-alternant hydrocarbons are given.

Rules which govern the change of the energy difference between the highest occupied and lowest unoccupied MO in a ring closure transformation are determined. An invariant of the number of bonding, non-bonding and antibonding MO's is proposed which can serve for a rough classification of conjugated hydrocarbons.

Parts of this work were published in: *Chem. Phys. Lett.* 16 (1972) 614; 17 (1972) 535; 20 (1973) 257; 24 (1974) 283; *Croat. Chem. Acta* 45 (1973) 423, 539; *J. Chem. Phys.* 59 (1973) 2772; 61 (1974) in press; *Tetrahedron* 20 (1973) 3449; *Naturwissenschaften* 60 (1973) 475; *Z. Naturforsch.* 29 b (1974) 80.

Examiners: Prof. M. Mirnik, Dr. D. Cvetković, Prof. N. Trinajstić, and

Prof. Z. Maksić

Oral examination: December 22, 1973.

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

(120 pages, 112 references, original in Croatian)

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**DCC-43 (Univ. Zagreb)**

1. Investigation of Topological  
Properties of Conjugated Hydrocarbons

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Conjugated hydrocarbons  
Graph theory  
Hückel theory  
Molecular orbitals  
Topology

DCC-44 (Univ. Zagreb)

Croat. Chem. Acta

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**The Study of Medium Influence upon Inhibitory Effect of Amines on Electrode Processes at the Mercury Electrode**

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Detailed research by means of DC- and AC-polarographic methods have been made to find out the influence of the kinds and concentration of acid, of technically important amines, aniline and cyclohexylamine at the dropping mercury electrode in the solution of perchloric, sulphuric and phosphoric acid. As indicating ions, the ions of cadmium and lead have been used.

The results of the research show that examined amines more inhibit the electrode process of cadmium and that the inhibition of electrode reaction depends on concentration of amines. Also, cyclohexylamine is a stronger inhibitor than aniline in electrode reactions of both used cations.

The degree of inhibition of studied amines, depending on medium, increases in sequence:

perchloric medium < sulphuric medium << phosphoric medium and decreases with decreasing ionic strength of medium.

The kinetic measurements indicate the dependence of rate of electrode processes on pH in the absence of amines as well as in their presence. The measured rate constant shows that by decreasing of pH the reversibility of electrode process increases with higher ionic strength, while at lower ionic strength with decreasing pH, it increases. The rate constants of electrode processes are also influenced by the change in ionic strength. Decreasing of the concentration of supporting electrolyte decreases the rate constants.

*Examiners:* Prof. I. Filipović, Prof. I. Piljac, Prof. B. Lovreček, and Prof. M. Mirnik.

*Oral examination:* March 14, 1974;

*Degree conferred:* April 26, 1974;

Thesis deposited at University Library, Zagreb and Faculty of Technology, University of Zagreb, 41000 Zagreb, Croatia.

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1. The Study of Medium Influence upon Inhibitory Effect of Amines on Electrode Processes at the Mercury Electrode

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AC-polarography  
—, inhibition studies with  
—, kinetic studies with  
Amines  
Aniline  
Cadmium  
Cyclohexylamine  
DC-polarography  
Inhibition of electrode reactions  
Inhibitory effect  
Kinetics electrode reactions  
Lead

DCC-45 (Univ. Zagreb)

Croat. Chem. Acta

CCACAA 46 (4) B7—B8 (1974)

**Investigation of the Electrode Processes on the Mercury in Aqueous Solutions of Cadmium(II) and Complexones of EDTA Type**

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As a model for metal-ligand interaction in natural aqueous systems the interaction between cadmium and complexones: nitrilotriacetic acid (NTA), ethylenediaminetetraacetic acid (EDTA), diethylenetriaminepentaacetic acid (DTPA), which form stable and inert chelates of  $z = -1, -2$  and  $-3$  charge at  $\text{pH} = 8$ , has been investigated. The mechanism of the electrochemical reduction of chelates has been determined comparing their polarographic behaviour.

The parameters of electrochemical reduction of Cd(II)-NTA chelate have been determined in aqueous solutions of  $\text{pH} = 8$ :  $D = (5.1 \pm 0.4) \times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$ ,  $z = -1$ ,  $k_{\text{c}}^{\circ} = 1.3$  and  $0.9 \times 10^{-4} \text{ cm s}^{-1}$  in 0.1 M NaCl and 0.1 M KCl, respectively,  $k_{\text{c}}^{\circ} = 0.161$  and  $0.125 \text{ cm s}^{-1}$ . The dissociation rate constant and the apparent stability constant were determined in various supporting electrolytes, e. g. in 0.03 M  $\text{CaCl}_2$  ( $\mu \approx 0.1 \text{ M}$ )  $k_{\text{d}} = 1.6 \pm 0.4 \text{ s}^{-1}$ ,  $\log K_{\text{cax}} = 5.85$ ; correction of the latter gives  $\log (K_{\text{cax}})_{\text{corr}} = 10.73$ .

Polarographic limiting current of Cd(II)-EDTA chelate at  $\text{pH} = 8$  is controlled by chemical reaction kinetics which precedes the electrode reaction and depends on concentration, kind and charge of the cations of the supporting electrolyte. The method for the investigation of the ionic pair formation in the bulk of the solution has been applied and the charge of the reducible species has been determined as  $z = -2$ .

Adsorption of EDTA anion on the mercury electrode has been investigated by means of capillary electrometer, streaming mercury electrode and a. c. bridge. It has been determined that the adsorption of the anion of di- and trisodium salt of EDTA occurs only in the potential range more positive than the electrocapillary maximum.

Cd(II)-DTPA chelate at  $\text{pH} = 9$  (most probable charge  $z = 3$ ) is not reduced within the polarographic potential range. Polarographic behaviour of Cd(II)-DTPA at  $\text{pH} = 6$  (most probable charge  $z = -2$ ) is similar to that of Cd(II)-EDTA at  $\text{pH} = 8$ . This confirms the proposed reduction mechanism of Cd(II)-EDTA, by which irreversible reduction of divalent anion is accelerated by preceding chemical reaction with the cations of the supporting electrolyte, the result of which is the formation of electroactive species of lower charge and energy of activation. Due to the larger concentration of the cations of the supporting electrolyte (Boltzmann distribution law) preceding chemical reaction most probably takes place in the electrical double layer on the outer Helmholtz plane.

*Examiners:* Dr. M. Branica, Prof. I. Filipović, Prof. M. Herak.

*Oral examination:* April 1, 1974.

(262 pages, 26 tables, 91 figures, 157 references, original in Croatian)

B. HERENDA-RASPOR

*DCC-45 (Univ. Zagreb)*

1. Investigation of the Electrode Processes on the Mercury in Aqueous Solutions of Cadmium (II) and Complexones of EDTA Type

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Cadmium(II)

—, complexes with complexones  
—, electrode processes of Complexones, EDTA type  
—, adsorption on mercury  
—, complexes with cadmium(II)

Electrochemistry

—, of cadmium(II)-complexones complexes



DCC-46 (Univ. Zagreb)

Croat. Chem. Acta

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**Hydroxytryptamines — the Synthesis and General  
Metabolism in Mammals**

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For biological investigations  $\beta$ -hydroxytryptamine and  $\beta$ -hydroxyserotonin were synthesized as crystalline, water soluble, creatinine sulphates.

The general metabolism of these compounds was investigated by using rat liver slices and the obtained metabolites were identified as corresponding indole-3-glycolic acids and indole-3-ethane diols. For this scope also 5-hydroxyindole-3-ethane diol, so far undescribed, was synthesized.

The relative rates of deamination of synthesized  $\beta$ -hydroxylated tryptamines were measured in the Warburg respirometer by using rat liver mitochondria as the source of monoamine oxidase and compared with the rates of deamination of  $\beta$ -nonhydroxylated tryptamines. At pH = 7.4 and final substrate concentration of  $0.66 \times 10^{-3}$  M it was found that the rates of deamination of  $\beta$ -hydroxylated tryptamines were lower than the rates of deamination of  $\beta$ -nonhydroxylated tryptamines.

The synthesized compounds were examined for four types of pharmacological activity: effect on smooth muscle *in vitro*, blood pressure, spontaneous respiration, and the resistance of respiratory pathways *in vivo*. It was found that  $\beta$ -hydroxylated tryptamines show similar, although weaker biological activity than  $\beta$ -nonhydroxylated tryptamines. The only difference is the pressor activity of  $\beta$ -hydroxytryptamine, which is identical with the activity of tryptamine.

The thesis was partly published in: *Croat. Chem. Acta* 44 (1972) 303.

Examiners: Dr. S. Kveder, Dr. A. Deljac and Prof. Z. Supek

Oral examination: May 8, 1974.

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

(80 pages, 7 tables, 13 figures, 93 references, original in Croatian).

V. PLAVŠIĆ

*DCC-46 (Univ. Zagreb)*

1.  $\beta$ -Hydroxytryptamines — the  
Synthesis and General Meta-  
bolism in Mammals

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$\beta$ -Hydroxytryptamine creatinine  
sulphate, synthesis of  
—, determination of general me-  
tabolism  
—, pharmacological activity of  
 $\beta$ -Hydroxyserotonin creatinine sul-  
phate, synthesis of  
—, determination of general me-  
tabolism  
—, pharmacological activity of

DCC-47 (Univ. Zagreb)

Croat. Chem. Acta

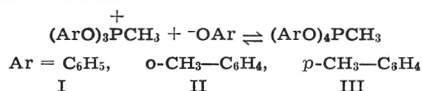
CCACAA 46(4) B11—B12 (1974)

### N.m.r. Studies of the Equilibration of Phosphonium Salts and Phosphoranes

I. Szele

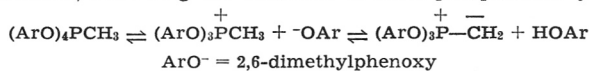
Harvard University, Cambridge, Mass., U.S.A. and Rugjer Bošković Institute, 41000 Zagreb, Yugoslavia

The interconversion between phosphonium salt and phosphorane was studied by n.m.r. methods.



The equilibrium constant for the reaction of each salt with aryloxide to give the phosphorane was found to be very large and its value could not be determined by the method used. Line shape analysis of the spectra provided rate constants for the dissociation of phosphoranes I—III. *Ortho*- and *para*-methyl group substitution in the ring influences the dissociation rates only by a small extent. The *p*-substituted phosphorane, III, dissociates faster than phosphorane I, presumably due to electronic stabilization of the developing phosphonium ion. The *o*-substituted phosphorane II, however, dissociates more slowly than phosphorane I, most likely because of steric hindrance to solvation.

Methyltetra(2,6-dimethylphenoxy)phosphorane, IV, was synthesized, too. It was found that the P—CH<sub>3</sub> protons exchange with deuterium in CDCl<sub>3</sub> solutions, indicating the existence of some phosphonium ylid.



At low temperatures the ring methyl groups of phosphorane IV cease to be n.m.r. equivalent and two separate signals ( $\Delta\delta = 0.69$ ) of equal intensities are observed at  $-57^\circ\text{C}$ . The temperature dependent n.m.r. behavior of phosphorane IV was shown, by comparison with that of dimethyltri(*o*-cresoxy)phosphorane, V, to be due to slow pseudorotation; the latter compound, V, was synthesized to allow this comparison. The steric crowding in the trigonal bipyramid of the »2,6-dimethylphenoxy« phosphorane seems to be large enough to account for this behavior. This is the first example for restricted pseudorotation of a tetraoxyphosphorane.

A part of this work was reported at the 2<sup>nd</sup> IUPAC Conference on Physical Organic Chemistry, Noordwijkerhout, the Netherlands, May 1974.

Examiners: Prof. D. E. Sunko, Prof. F. H. Westheimer, Prof. C. F. Wilcox, Jr.

Oral examination: June 18, 1974.

Thesis deposited at the University of Zagreb, Faculty of Natural Sciences and Mathematics, and at the Rugjer Bošković Institute, Zagreb. (144 pages, 5 tables, 35 figures, 126 references, original in English with a detailed summary in Croatian).

I. SZELE

DCC-47 (*Univ. Zagreb*)

1. N.m.r. Studies of the Equilibration of Phosponium Salts and Phosphoranes

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N.m.r. spectra, line shape analysis of  
Phosponium salts  
Phosphoranes, pentacovalent  
Pseudorotation, inhibited

MCC-65 (Univ. Zagreb)

Master of Science Thesis

Croat. Chem. Acta

CCACAA (46) B13—B14 (1974)

**The Sulphur-34 Isotope Effect in the Reaction of  
2-Phenylethyldimethylsulphonium Bromide with Sodium Ethoxide  
in Ethyl Alcohol and the Reduction of the Sulphonium  
Salt with Lithium Aluminium Hydride**

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The reaction of 2-phenylethyldimethylsulphonium bromide with sodium ethoxide was studied in ethyl alcohol solution. In the reaction dimethylsulphide was produced, this was then oxidized by oxygen at 1000 °C to sulphur dioxide.

The sulphur-34 isotope effect was measured and it was found to be 1.26‰ at 20.1 °C. The maximum sulphur-34 isotope effect in the reaction of sulphonium salts for breaking C—S bond was calculated to be from 1.51 to 1.57‰ at 25 °C.

The experimental results show that the sulphur-34 isotope effect in the ethyl alcohol solution is about 2/3 the theoretical, but in the correlation with the value of the sulphur-34 isotope effect in the aqueous solution it can be concluded that both sulphur-34 isotope effects are the same, which means that the solvent has no influence on the mechanism of the reaction. The experimental value of the sulphur-34 isotope effect indicated the concerted mechanism of this reaction.

In studying the reaction of deuterated trimethylsulphonium bromide with lithium aluminium hydride, methane was isolated, and analysed by mass spectrometry. The mass spectrum contained an intense mass of 19 units corresponding to CHD<sub>3</sub>, but no detected methane of the formula CH<sub>2</sub>D<sub>2</sub>. This experimental result suggests that possibly simple displacement is occurring:



as the reaction mechanism.

The thesis was partly published in: *J. Org. Chem.* 33 (1968) 2526.

Examiners: Prof. S. Ašperger, Dr. S. Borčić, and Prof. H. Iveković.

Oral examination: February 15, 1967.

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(80 pages, 3 tables, 5 figures, 87 references, original in Croatian).

D. HEGEDIĆ

*MCC-65 (Univ. Zagreb)*

1. The Sulphur-34 Isotope Effect in the Reaction of 2-Phenylethyldimethylsulphonium Bromide with Sodium Ethoxide in Ethyl Alcohol and the Reduction of the Sulphonium Salt with Lithium Aluminium Hydride

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Isotope effects,  $^{34}\text{S}$   
2-Phenylethyldimethylsulphonium bromide,  
—, reaction with sodium ethoxide  
—, reduction with LAH  
Sulphur-34, isotope effect

MCC-66 (Univ. Zagreb)

Master of Science Thesis

Croat. Chem. Acta

CCACAA 46 (4) B15—B16 (1974)

**Study of the Cyclization of 2-(3-Butenyl)-2-cyclohexenyl  
Derivatives**

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The aim of this work was to obtain additional information on the mechanism of nonenzymic biogenetic-like olefinic cyclization. The following compounds were prepared: 2-(3-butenyl)-3-methyl-2-cyclohexenyl *p*-nitrobenzoate (Ia), 2-(3-butenyl)-3-methyl-2-cyclohexenyl-1-*d*<sub>1</sub> *p*-nitrobenzoate (Ib) and 2-(3-butenyl)-3-methyl-1-methyl-*d*<sub>3</sub>-2-cyclohexenol (II).

Solvolysis of Ia in 97% 2,2,2-trifluoroethanol (TFE) gave about 34% of cyclic products, but solvolysis of this ester in 80% ethanol gave exclusively non-cyclic products. The secondary  $\alpha$ -deuterium isotope effect in the solvolysis of Ib in 97% TFE is slightly decreased ( $k_H/k_D = 1.14$ ).

The study of the cyclization of alcohol II in anhydrous formic acid confirmed Johnson's hypothesis which implies the formation of a resonance stabilized cation as intermediate.

On the basis of obtained results a cyclization mechanism of 2-(3-butenyl)-2-cyclohexenol derivatives, including the formation of a cationic intermediate with a resonance stabilized allylic cation, can be proposed. Using the INDO SCF MO method, the energies of different conformers of the 3-methyl derivative of the cited cation were calculated in order to predict the products that are formed in the cyclization process. The results showed that of the two possible effects, *i. e.* steric and electronic, the first is the predominant one, resulting in the formation of cyclic products without an angular methyl group. This result is in accordance with the proposed cyclization mechanism, which does not include a concerted, but a stepwise process.

*Examiners:* Prof. D. Sunko, Prof. S. Borčić and Dr. T. Cvitaš

*Oral examination:* November 13, 1974.

Thesis deposited at the University of Zagreb.

(135 pages, 9 tables, 1 figure, 120 references, original in Croatian)

M. LADIKA

*MCC-66 (Univ. Zagreb)*

1. Study of the Cyclization of  
2-(3-Butenyl)-2-Cyclohexenyl  
Derivatives

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Croatia, Yugoslavia

Allylic cations, conformation of  
2-Cyclohexen-1-ol, derivatives,  
solvolysis of

Isotope effects, deuterium, secondary

Molecular orbital, intermediate  
neglect of differential overlap  
Solvolysis



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BCC-1273

V. Bonačić and J. Koutecký

Department of Chemistry, The Johns Hopkins University, Baltimore, Maryland 21218 and Belfer Graduate School of Science, Yeshiva University, New York 10033

**Convergence Difficulties in the Hartree-Fock Procedure for the PPP Model of Alternant Hydrocarbons***Int. J. Quant. Chem.* 5S (1971) 137.

BCC-1274

O. Carević and N. Čerlek

Department of Biology, Institute »Ruder Bošković« and Department of Surgery, »Dr Mladen Stojanović« Hospital, Zagreb, Yugoslavia

**The Inhibitory Effect of Oxytetracycline on the Glucose Degradation in Human Erythrocytes***Enzymologia* 41 (1971) 53.

BCC-1275

D. Hace and M. Bravar

Institute of Organic Chemical Technology, Faculty of Technology, University of Zagreb, Croatia, Yugoslavia

**Friedel-Crafts and Related Reactions on Poly(Vinyl Chloride)***J. Polym. Sci. Part C* No 33 (1971) 325.

BCC-1276

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**On Convergence Difficulties in the Iterative Hartree-Fock Procedure***J. Chem. Phys.* 55 (1971) 2408.

BCC-1277

J. Koutecký and V. Bonačić

Belfer Graduate School of Science, Yeshiva University, New York, New York 10033, USA and Department of Chemistry, The Johns Hopkins University, Baltimore, Maryland 21218, USA

**Direct Minimization of Hartree-Fock Energy for Alternant Hydrocarbons in the PPP Model***Chem. Phys. Lett.* 10 (1971) 401.

BCC-1278

S. Kveder, N. Revelante, N. Smodlaka and A. Škrivanić

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

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BCC-1279

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i N. S. Enikolopyan

Institut khimičeskoj fiziki Akademii Nauk SSSR, Moskva

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BCC-1280

E. Reiner

Institute for Medical Research and Occupational Health,  
Yugoslav Academy of Sciences and Arts, Zagreb, Yugoslavia**Spontaneous Reactivation of Phosphorylated and Carbamylated Cholinesterases***Bull. W. H. O.* **44** (1971) 109.

1972

BCC-1281

J. E. Bloor and Z. B. Maksić

Chemistry Department, The University of Tennessee, Knoxville,  
Tennessee 37916**Calculation of the Second Moments of the Electronic Charge Distribution and Molecular Quadrupole Moments of Some Fluorine Containing Compounds by the CNDO/2D Method***J. Chem. Phys.* **57** (1972) 3572.

BCC-1282

D. Cvetković, I. Gutman, and N. Trinajstić

Faculty of Electrical Engineering, University of Belgrade, Serbia,  
Yugoslavia and Institute Ruđer Bošković, P. O. Box 1016, 41001 Zagreb,  
Croatia, Yugoslavia**Kekulé Structures and Topology***Chem. Phys. Lett.* **16** (1972) 614.

BCC-1283

R. Despotović and J. Tomić

Department of Physical Chemistry, »Ruđer Bošković« Institute, Zagreb  
(Croatia, Yugoslavia)**Heterogeneous Exchange-Processes. XXI. TII—<sup>131</sup>I Exchange***Kolloid-Z. Z. Polym.* **250** (1972) 956.

BCC-1284

Đ. Deur-Šiftar and V. Mitrović

INA-Institute, Zagreb, Yugoslavia and JUGOVINIL, Split, Yugoslavia

**Determination Thermal Stability of pVC by Reaction Gas Chromatography***Chromatographia* **5** (1972) 573.

BCC-1285

H. L. Goering, J. V. Clevenger, and K. Humski

Department of Chemistry, University of Wisconsin, Madison Wisconsin 53706

**Preparation and Stereochemistry of 1-Methyl-2-methylenebenzonorbornene and 1,2-Dimethyl-2-benzonorbornenyl Derivatives***J. Org. Chem.* **37** (1972) 3019.

BCC-1286

H. Guesten and L. Klasinc

Institut für Strahlenchemie, Kernforschungszentrum Karlsruhe,  
Karlsruhe, Germany**Conductance of an Intermolecular Charge-Transfer Complex  
within an Ion Pair***J. Phys. Chem.* **76** (1972) 2452.

BCC-1287

J. N. Herak and M. Paić

Institute »Ruder Bošković« and Institute of Physics of the University,  
Zagreb, Croatia, Yugoslavia**EPR Study of Cadmium Sulphide-Manganese Sulphide Systems  
Prepared by Coprecipitation with Ammonium Sulphide***J. Phys. Chem. Solids* **33** (1972) 1159.

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**Deuterium Isotope Effects in Mass Spectrometry. Mechanism of  
Formation of the  $[C_6H_6S]^+$  Ion in the Decomposition of *S*-Phenyl  
Methylthiocarbamate***Org. Mass Spectrom.* **7** (1973) 1415.

BCC-1365

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Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia and Laboratory  
of Analytical Chemistry, Faculty of Science, University of Zagreb,  
Zagreb, Croatia, Yugoslavia**Mass Spectral Studies of Some Complexes of Niobium(V) and  
Tantalum(V) with Chloro, Alkoxy, Acetylacetonato or  
Salicylaldehydato Ligands***Org. Mass Spectrom.* **7** (1973) 1357.

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B. Svetličić and K. Wilhelm

Andrija Stampar School of Public Health, Medical Faculty, University of  
Zagreb and Institute for Medical Research, Yugoslav Academy of Sciences  
and Arts, Zagreb**Methods of Measuring Exposure to Anticholinesterase Insecticides***Arh. Hig. Rada Toksikol.* **24** (1973) 357.

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N. Šegudović, Gj. Deželić, and D. Fleš

Department of Physical Chemistry, Institute »Ruder Bošković«, Department  
of Biological Chemistry, Andrija Stampar School of Public Health, Faculty  
of Medicine, University of Zagreb, Zagreb, Yugoslavia and Research and  
Development Institute INA, Zagreb, Yugoslavia**Light Scattering on Optically Active Polythiol Esters.  
Determination of Molecular Weight and Optical Anisotropy of  
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Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia

**Novel Azabicyclo [4,2,1] Nonanes from Anhydrodihydroneucleosides***J. Chem. Soc. D* (1973) 495.

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M. Škrinjarić-Špoljar, V. Simeon, and E. Reiner  
Institute for Medical Research, Yugoslav Academy of Sciences and Arts,  
Zagreb, Croatia (Yugoslavia)

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Acetylcholinesterase and Cholinesterase**

*Biochim. Biophys. Acta* **315** (1973) 363.

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V. Šunjić, F. Kajfež, I. Štromar, N. Blažević,  
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Compagnia di Ricerca Chimica SA., Chiasso, Switzerland and Institute of  
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1,4-Benzodiazepin-2-ones Containing  $\alpha$ -Amino Acids as a Part  
of the 1,4-Diazepine Ring**

*J. Heterocycl. Chem.* **10** (1973) 591.

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V. Šunjić, F. Kajfež, M. Štromar, N. Blažević,  
M. Oklobdžija

CRC, Compagnia di Ricerca Chimica, Chiasso, Switzerland, Institut za  
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**NMR Study of Hexaminium Salt Formation of  $\alpha$ -Bromo-N-  
-Methyl-Phenylacetamide**

*Bull. Sci. Cons. Acad. Sci. Arts RSF Yougoslavie Sect. A* **18**  
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CRC, Compagnia di Ricerca Chimica, Chiasso, Switzerland and Institute of  
Organic Chemistry and Biochemistry, University of Zagreb, Zagreb

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3-(S)-Methyl-5-phenyl-7-Chloro-1,3-dihydro-2H-1,4-benzo-  
diazepine-2-one**

*Acta Pharm. Jugoslav.* **23** (1973) 213.

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K. Wilhelm, R. Pleština, i B. Svetličić

Institut za medicinska istraživanja i medicinu rada JAZU i Škola narodnog  
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**Aktivnost kolinesteraza u krvi radnika izloženih organskom  
fosforom insekticidu Ekatinu**

*Arh. Hig. Rada Toksikol.* **24** (1973) 107.

BCC-1374

K. Wilhelm and E. Reiner

Institute for Medical Research and Occupational Health, Yugoslav Academy  
of Sciences and Arts, Zagreb, Yugoslavia

**Effect of Sample Storage on Human Blood Cholinesterase  
Activity after Inhibition by Carbamates**

*Bull. W. H. O.* **48** (1973) 363

BCC-1375

K. Wilhelm, M. Vandekar, and E. Reiner

Institute for Medical Research and Occupational Health, Yugoslav Academy  
of Sciences and Arts, Zagreb, Yugoslavia

**Comparison of Methods for Measuring Cholinesterase Inhibition  
by Carbamates**

*Bull. W. H. O.* **48** (1973) 41.

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M. Wrischer

Ruder Bošković Institute, Zagreb, Yugoslavia

**Protein Crystalloids in the Stroma of Bean Plastids***Protoplasma* **77** (1973) 141.

BCC-1377

M. Wrischer

Ruder Bošković Institute, Zagreb, Yugoslavia

**Ultrastructural Changes in Isolated Plastids. I. Etioplasts***Protoplasma* **78** (1973) 291.

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Ruder Bošković Institute, Zagreb, Yugoslavia

**Ultrastructural Changes in Isolated Plastids. II. Etio-Chloroplasts***Protoplasma* **78** (1973) 417.

BCC-1379

M. Wrischer

Ruder Bošković Institute, Zagreb, Yugoslavia

**The Effect of Ethionine on the Fine Structure of Bean Chloroplasts***Cytobiologie* **7** (1973) 211.

BCC-1380

M. Zebec, D. Sinković, N. Deželić, D. Jušić,  
Gj. Deželić, and B. PendeAndrija Štampar School of Public Health, Medical Faculty, Zagreb and  
Institute of Immunology, Zagreb**Gel Chromatography of the Lipopolysaccharide from *Salmonella Typhi* on the Sepharose 4B Gel***Acta Pharm. Jugoslav.* **23** (1973) 59.

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E. Zissis, H. W. Diehl, H. G. Fletcher, Jr., and  
N. PravdićNational Institute of Arthritis, Metabolism and Digestive Diseases, National  
Institutes of Health, Public Health Service U. S. Department of Health,  
Education and Welfare, Bethesda, Maryland 20014 (U. S. A.) and Department  
of Organic Chemistry and Biochemistry, »Ruder Bošković« Institute,  
Zagreb, Croatia, Yugoslavia**Dicyclohexylammonium Salts for the Isolation and Characterization  
of Aldonic Acids***Carbohydr. Res.* **26** (1973) 323.

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V. Žutić, P. Gerard, E. Nicolas and L. Gierst  
Faculté des Sciences, Université Libre, Bruxelles (Belgium)**Heterocoagulation Between Colloidal Particles and Charged  
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Characterization and Kinetics of the Aquation**  
*Inorg. Chem.* **13** (1974) 57.

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A. Bakač and M. Orhanović  
Institute »Ruder Bošković«, Bijenička 54, Zagreb, Yugoslavia  
**Characterization of the Geometric Isomers of the Tetra-  
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*Z. Naturforsch. B* **29** (1974) 134.

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M. Biruš, W. L. Reynolds, M. Pribanić, and  
S. Ašperger  
Department of Chemistry, Faculty of Pharmacy and Biochemistry,  
University of Zagreb, and Institute »Ruder Bošković«, Zagreb, Croatia,  
Yugoslavia  
**Kinetics and Mechanism of Base Hydrolysis of (Dimethyl  
Sulphoxide) Pentaaminecobalt(III) Ions**  
*Proc. XVI Int. Conf. Coord. Chem.* (1974) 3. 6.

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Z. Bradić, D. Pavlović, I. Murati, and S. Ašperger  
Department of Chemistry, Faculty of Pharmacy and Biochemistry,  
University of Zagreb and Institute »Ruder Bošković«, Zagreb, Croatia,  
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*J. Chem. Soc. Dalton Trans.* (1974) 344.

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Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia and College of  
William and Mary, Williamsburg, Virginia 23185, U. S. A.  
**Co-ordination Complexes of Niobium and Tantalum. Part XV.  
Sulphoxide Complexes of Oxobis(oxalato)niobates(V)**  
*J. Chem. Soc. Dalton Trans.* (1974) 165.

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O. Carević, V. Šverko, M. Boranić, and V. Prpić  
Department of Experimental Biology and Medicine, Ruder Bošković  
Institute, and Research Department »Pliva«, Pharmaceutical and Chemical  
Works, P. O. Box 1016, 41001 Zagreb, (Yugoslavia)  
**Effect of Glorafur on Acid Phosphatase Activity in the Liver  
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*Experientia* **30** (1974) 241.

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D. Cvetković, I. Gutman, and N. Trinajstić  
Faculty of Electrical Engineering, University of Belgrade, P. O. B. 316,  
11001 Belgrade, Serbia, Yugoslavia and Institute »Ruder Bošković«, P. O. B.  
1016, 41001 Zagreb, Croatia, Yugoslavia  
**Graph Theory and Molecular Orbitals. IX. On the Stability  
of Cata-Condensed Hydrocarbons**  
*Theor. Chim. Acta* **34** (1974) 129.



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V. Čaplar, V. Šunjić, and F. Kajfež

CRC, Compagnia di Ricerca Chimica SA., Chiasso, Switzerland, Institute of Organic Chemistry and Biochemistry, University of Zagreb, and Institute for the Control of Drugs, Zagreb

**N<sup>1</sup>-Substitution in 4(5)-Nitroimidazole. IV. New Synthesis of N<sup>1</sup>-Ethylsulphonyl-Ethyl-2-Methyl-5-Nitroimidazole***J. Heterocycl. Chem.* **11** (1974) 681.

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V. Čaplar, V. Šunjić, F. Kajfež, and J. Kuffinec

CRC, Compagnia di Ricerca Chimica SA., Chiasso, Switzerland, Institute of Organic Chemistry and Biochemistry, University of Zagreb and Institute for the Control of Drugs, Zagreb

**Physico-Chemical Properties and Identification Methods of Tinidazole***Acta Pharm. Jugoslav.* **24** (1974) 147.

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B. Čeluška and S. Popović

Institute »Ruder Bošković«, 41001 Zagreb, P. O. B. 1016, Yugoslavia

**The Synthesis of In<sub>5</sub>Se<sub>6</sub> and In<sub>2</sub>Se from InSe by Zone-Melting Process***J. Phys. Chem. Solids* **35** (1974) 287.

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Electrochemistry Laboratory, Ruder Bošković Institute, Zagreb, Croatia (Yugoslavia)

**Measurement of Rates of Chemical Reactions Coupled to Electron Transfer by Cyclic Chronopotentiometry***J. Electroanal. Chem.* **49** (1974) 415.

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Electrochemistry Laboratory, Ruder Bošković Institute, Zagreb, Croatia (Yugoslavia)

**An Investigation into the Reaction Mechanism of Uranium(VI) Reduction in Acidic Solutions by Cyclic Chronopotentiometry***J. Electroanal. Chem.* **49** (1974) 421.

## BCC-1396

Č. Čosović, Z. Jandrić, and M. Proštenik

Zavod za kemiju i biokemiju, Medicinskog fakulteta Sveučilišta u Zagrebu, 41000 Zagreb, Salata 3

**Lipids of Higher Fungi. I. Mycoglycolipids, a New Glass of Complex Lipids of Mushrooms***Bull. Sci. Cons. Acad. Sci. Arts RSF Yougoslavie Sect. A* **19** (1974) 2.

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M. Dikšić, D. K. McMillan, and L. Yaffe

Department of Chemistry, McGill University, Montreal, Quebec, Canada

**Nuclear Charge Dispersion in Mass Chain 130—135 from the Fission of <sup>238</sup>U by Medium-Energy Protons***J. Inorg. Nucl. Chem.* **36** (1974) 7.

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M. Dikšić, P. Strohal, and I. Šlaus

Institute »Ruder Bošković«, Zagreb, Yugoslavia

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BCC-1399

B. Dugonjić, L. Kolačni-Babić, H. Krnjević,  
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fakulteta Sveučilišta, Zagreb i Farmakološki laboratorij »Pliva«, Zagreb**Lipotropic Action of Lipocain Compared to Other Lipotropic  
Factors***Bull. Sci. Cons. Acad. Sci. Arts RSF Yougoslavie Sect. A* **19**  
(1974) 129.

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M. Eckert-Maksić and Z. B. Maksić

Institute »Ruder Bošković«, 41001 Zagreb, Croatia, Yugoslavia

**Maximum Overlap Hybridization in Norbornane and Some  
Related Molecules***J. Mol. Struct.* **22** (1974) 445.

BCC-1401

V. Fintić and J. Bešić

Zavod za ispitivanje i kontrolu lijekova SRH, Zagreb

**Određivanje atropina u prisutnosti pralidoksim-klorida metodom  
plinske kromatografije***Acta Pharm. Jugoslav.* **24** (1974) 157.

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D. Grdenić, B. Kamenar, B. Korpar-Čolig,  
M. Sikirica, and G. JovanovskiLaboratory of General and Inorganic Chemistry, Faculty of Science,  
University of Zagreb, 41001 Zagreb, P. O. Box 153, Yugoslavia**Tetrakis (trifluoroacetoxymcury) methane and Tetrakis  
(acetoxymcury) methane as the Reaction Products of Hofmann's  
Base with the Corresponding Acid: X-Ray Crystallographic  
Evidence***J. Chem. Soc. D* (1974) 646.

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B. Grgas-Kužnar, Vl. Simeon, and O. A. Weber

Laboratory of Analytical and Physical Chemistry, Institute for Medical  
Research and Occupational Health, Yugoslav Academy of Sciences and  
Arts, 41001 Zagreb, Croatia, Yugoslavia**Complexes of Adrenaline and Related Compounds with Ni<sup>2+</sup>, Cu<sup>2+</sup>,  
Zn<sup>2+</sup>, Cd<sup>2+</sup>, and Pb<sup>2+</sup>***J. Inorg. Nucl. Chem.* **36** (1974) 2151.

BCC-1404

Lj. Grlić

Yugoslav Lexicographical Institute, Zagreb, Yugoslavia

**Identification of Cannabis Users by Detecting Cannabinoids  
in Biological Media***Acta Pharm. Jugoslav.* **24** (1974) 63.

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CRC, Compagnia di Ricerca Chimica SA., Chiasso, Switzerland, Institute of Organic Chemistry and Biochemistry, University of Zagreb, and Institute for the Control of Drugs, Zagreb

**N<sup>1</sup>-Substitution in 4(5)-Nitroimidazole. IV. New Synthesis of N<sup>1</sup>-Ethylsulphonyl-Ethyl-2-Methyl-5-Nitroimidazole***J. Heterocycl. Chem.* **11** (1974) 681.

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CRC, Compagnia di Ricerca Chimica SA., Chiasso, Switzerland, Institute of Organic Chemistry and Biochemistry, University of Zagreb and Institute for the Control of Drugs, Zagreb

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Institute »Ruder Bošković«, 41001 Zagreb, P. O. B. 1016, Yugoslavia

**The Synthesis of In<sub>5</sub>Se<sub>8</sub> and In<sub>2</sub>Se from InSe by Zone-Melting Process***J. Phys. Chem. Solids* **35** (1974) 287.

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Electrochemistry Laboratory, Ruder Bošković Institute, Zagreb, Croatia (Yugoslavia)

**Measurement of Rates of Chemical Reactions Coupled to Electron Transfer by Cyclic Chronopotentiometry***J. Electroanal. Chem.* **49** (1974) 415.

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Electrochemistry Laboratory, Ruder Bošković Institute, Zagreb, Croatia (Yugoslavia)

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Zavod za kemiju i biokemiju, Medicinskog fakulteta Sveučilišta u Zagrebu, 41000 Zagreb, Salata 3

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M. Dikšić, D. K. McMillan, and L. Yaffe

Department of Chemistry, McGill University, Montreal, Quebec, Canada

**Nuclear Charge Dispersion in Mass Chain 130—135 from the Fission of <sup>238</sup>U by Medium-Energy Protons***J. Inorg. Nucl. Chem.* **36** (1974) 7.

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H. Güsten, L. Klasinc, V. Kramer, and J. Marsel  
Institute »Ruder Bošković«, Zagreb, Yugoslavia, Institut für Radiochemie  
Kernforschungszentrum, Karlsruhe, Germany, »J. Stefan« Institute,  
University of Ljubljana, Yugoslavia

**Correlation of Fragmentation Modes of Substituted Stilbenes  
under Electron Impact**

*Adv. Mass Spectrom.* **6** (1974) 79.

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H. Güsten, L. Klasinc, V. Kramer, and J. Marsel  
Institut für Radiochemie, Kernforschungszentrum Karlsruhe, Germany,  
Institute »Ruder Bošković«, Zagreb, Yugoslavia and »J. Stefan« Institute,  
University of Ljubljana, Yugoslavia

**Mass Spectra of Monosubstituted *trans* Stilbenes**

*Org. Mass Spectrom.* **8** (1974) 323.

## BCC-1407

I. Gutman

Institute »Ruder Bošković«, P. O. B. 1016, 41001 Zagreb, Croatia, Yugoslavia

**Bound for Total  $\pi$ -Electron Energy**

*Chem. Phys. Lett.* **24** (1974) 283.

## BCC-1408

I. Gutman

Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia

**On the Number of Antibonding MO's in Conjugated Hydrocarbons**

*Chem. Phys. Lett.* **26** (1974) 85.

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I. Gutman

Institute »Ruder Bošković«, Zagreb, Croatia, Yugoslavia

**Estimating the  $\pi$ -Electron Energy of Very Large Conjugated  
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*Naturwissenschaften* **61** (1974) 216.

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I. Gutman, J. V. Knop, and N. Trinajstić

Institute »Ruder Bošković«, Zagreb, Yugoslavia and Rechenzentrum der  
Universität Düsseldorf

**A Graph-theoretical Analysis of the HOMO-LUMO Separation  
in Conjugated Hydrocarbons**

*Z. Naturforsch. B* **29** (1974) 80.

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Institute »Ruder Bošković«, P. O. B. 1016, Zagreb, Croatia, Yugoslavia

**Violation of the Dewar-Longuet-Higgins Conjecture**

*Z. Naturforsch. A* **29** (1974) 1238.

## BCC-1412

J. W. Hayes, I. Ružić, and D. E. Smith

Department of Chemistry, Northwestern University, Evanston, Ill. 60201  
(U. S. A.)

**Fundamental Harmonic A. C. Polarography with Disproportionation  
Following the Charge Transfer Step. Theory and Experimental  
Results with the U(VI)/U(V) Couple**

*J. Electroanal. Chem.* **51** (1974) 245.

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Department of Chemistry, Northwestern University, Evanston, Ill. 60201  
(U. S. A.)**Fundamental Harmonic A. C. Polarography with Irreversible Dimerization Following the Charge Transfer Step. Theory and Experimental Results with the Benzaldehyde System***J. Electroanal. Chem.* **51** (1974) 269.

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J. N. Herak and C. A. McDowell

Department of Chemistry, University of British Columbia, Vancouver,  
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## BCC-1415

M. Herceg and J. Fischer

Institute »Ruder Bošković«, 41001 Zagreb, Croatia, Yugoslavia and  
Laboratoire de Cristalochimie, Institut de Chimie, Université Louis  
Pasteur, B. P. 296/R3, 67008 — Strassbourg Cedex, France**Structure Cristalline du Dichlorobis-(N,N-diméthylacétamide) zinc(II)***Acta Crystallogr. Sect. B* **30** (1974) 1289.

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S. Hiršl-Starčević, Z. Majerski, and D. E. Sunko

Ruder Bošković Institute, 41001 Zagreb, Croatia, Yugoslavia and  
Department of Chemistry, Indiana University, Bloomington, Indiana 47401**Stereochemistry of the Solvolysis of Mentyl Tosylate. An Example of Retained Chair Conformation in the Transition State***J. Amer. Chem. Soc.* **96** (1974) 3659.

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K. Humski, V. Sendijarević, and V. J. Shiner, Jr.

Faculty of Technology, University of Zagreb, 44000 Sisak, Croatia, Yugo-  
slavia, Institute »Ruder Bošković«, 41000 Zagreb, Croatia, Yugoslavia, and  
Department of Chemistry, Indiana University, Bloomington, Indiana 47401**Stereochemistry of Olefine Formation in Cyclopentyl Brosylate Solvolysis***J. Amer. Chem. Soc.* **96** (1974) 6187.

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INA — Institute, Zagreb, Croatia, Yugoslavia

**Gas Chromatographic Determination of Inorganic Gases in High Purity Ethylene***Chromatographia* **7** (1974) 19.

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Ruder Bošković Institute, 41001 Zagreb, Yugoslavia

**Sulfuric Acid Catalyzed Rearrangements of 1- and 3-Homoadamantanol***J. Org. Chem.* **39** (1974) 651.

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D. Keglević, B. Ladešić, O. Hadžija, J. Tomašić,  
Z. Valiger, M. Pokorny, and R. Naumski

Tracer Laboratory, Institute »Ruder Bošković«, Zagreb and Research  
Department, PLIVA, Pharmaceutical and Chemical Works, Zagreb

**Isolation and Study of the Composition of a Peptidoglycan****Complex Excreted by the Biotin-Requiring Mutant of*****Brevibacterium Divaricatum* NRRL-2311 in the Presence of****Penicillin**

*Eur. J. Biochem.* **42** (1974) 389.

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K. Kljaić, Lj. Bzik, and M. Proštenik

Zavod za kemiju i biokemiju, Medicinski fakultet, Sveučilište u Zagrebu,  
41001 Zagreb, Salata 3

**Studies in the Sphingolipids Series. XXXVI. Synthesis of****DL-erythro-1,3-Dihydroxy-2-Amino-Hexadecane(racem.****C<sub>16</sub>-Dihydrosphingosine)**

*Bull. Sci. Cons. Acad. Sci. Arts RSF Yougoslavie Sect. A* **19**  
(1974) 177.

## BCC-1422

J. V. Knop, N. Trinajstić, and T. Živković

Rechenzentrum, Universität Düsseldorf, F.R. Germany and Institute  
»Ruder Bošković«, P. O. B. 1016, 41001 Zagreb, Croatia, Yugoslavia

**A Graphical Study of Positional Isomers Containing Bivalent Sulphur**

*Collect. Czech. Chem. Commun.* **39** (1974) 2431.

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B. Kojić-Prodić, R. Liminga, M. Šljukić, and  
Ž. Ružić-Toroš

Ruder Bošković Institute, 41001 Zagreb, P. O. Box 1016, Yugoslavia

**Molecular Crystal Structure of 5,6-Dihydro-2-thiouridine,****C<sub>8</sub>H<sub>14</sub>N<sub>2</sub>O<sub>5</sub>S**

*Acta Crystallogr. Sect. B* **30** (1974) 1550.

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B. Kojić-Prodić, Ž. Ružić-Toroš, D. Grdenić,  
and Lj. Golić

Institute »Ruder Bošković«, P. O. Box 1016, 41001 Zagreb, Yugoslavia

**The Crystal Structure of Dioxobis-(1,3-diphenylpropane-dionatato)****molybdenum(VI), (C<sub>15</sub>H<sub>11</sub>O<sub>2</sub>)<sub>2</sub>MoO<sub>2</sub>**

*Acta Crystallogr. Sect. B* **30** (1974) 300.

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J. Koller, A. Ažman, and N. Trinajstić

Chemical Institute »Boris Kidrič«, P. O. B. 380, 61001 Ljubljana, Slovenia,  
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Croatia, Yugoslavia

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