

UDC 54

Coden: CCACAA

YU ISSN 0011—1643

D O C U M E N T A C H E M I C A Y U G O S L A V I C A

CROATICA CHEMICA ACTA

Vol. 57

INDEX

Z A G R E B
YUGOSLAVIA
1984

Croat. Chem. Acta

CCACAA

CROATICA CHEMICA ACTA

Adresa redakcije

Address of the Editorial Board

CROATICA CHEMICA ACTA
19 Marulićev trg, Zagreb, Croatia, Yugoslavia

REDAKCIJSKI ODBOR — EDITORIAL BOARD

Glavni urednik — Editor-in-Chief
Siniša Maričić

Pomoćni urednici — Assistant Editors
Mladen Biruš i Marijan Pribanić

Tajnik — Secretary
Dina Keglević

Pomoćni tajnik — Assistant Secretary
Vera Mikulčić

Članovi odbora — Members

M. Eckert-Maksić, B. Grabarić, L. Klasinc, Z. Konrad, Ž. Kučan, Z. B. Maksić, B. Matković, Z. Meić, I. Piljac, N. Pravdić, V. Pravdić, M. Proštenik, E. Reiner, B. Ruščić, Vl. Simeon, V. Šunjić, B. Tamhina, Đ. Težak i N. Trinajstić

REDAKCIJSKI SAVJET — ADVISORY BOARD

K. Balenović, A. Bezjak, A. Despić, Gj. Deželić, M. Deželić, I. Filipović, V. Gall, D. Grdenić, H. Iveković, B. Kamenar, O. Lahodny-Šarc, B. Lovreček, D. Maljković, P. Mildner, M. Mirnik, M. Proštenik, M. Randić, P. Strohal, D. Sunko, V. Škarić i M. Tišler

CONTENTS

ORIGINAL SCIENTIFIC PAPERS

GENERAL AND THEORETICAL CHEMISTRY

S. El-Basil: An Easy Combinatorial Algorithm for the Construction of Sextet Polynomials of Cata-Condensed Benzenoid Hydrocarbons	1
S. El-Basil: Molecular Topology and Molecular Properties. I. »Sequence« Labels of Cata-Condensed Benzenoid Hydrocarbons Containing up to Five Rings	21
S. El-Basil: On a Graph-Theoretical Approach to Kekulé Structures. Novel Identities of Sextet Polynomials and a Relation to Clar's Sextet Theory	47
M. Hodošek, D. Kocjan, and T. Šolmajer: <i>Ab Initio</i> MO Study of Hydrogen Bonded Complex: Noradrenaline-Formic Acid	65
M. Topić and A. Moguš-Milanković: A Multiple Thermal Analysis of Ammonium Heptamolybdate Tetrahydrate	75
A. Julg and B. Deprick: Theoretical Study of Adsorption of Carbonyl Compounds on Ionic Crystals: I. Formaldehyde, Glyoxal, <i>o</i> - and <i>p</i> -Benzoinone on the (100) Face of Sodium Chloride	85
D. Težak, F. Strajnar, D. Šarčević, O. Milat, and M. Stubičar: Solid/Liquid Equilibria in Aqueous Systems of Dodecyl Benzene Sulphonate and Alkaline Earth Ions	93
S. K. Dua, V. Kapur, and S. K. Sahni: Titanyl(IV), Zirconyl(IV), Hafnyl(IV) and Uranyl(VI) Complexes of Terdentate Benzoyl Hydrazones	109
Lj. Tušek-Božić and B. Božić: Conductance Study of Ion-Pairing of Alkali Picrate and Tetraphenylborate Complexes with Some Macrocyclic Polyethers in Methanol	119
D. Dasić, M. E. Marcondes Helene, L. W. Reeves, and M. Szarka: Micelle Forms in Lyotropic Nematics and Cholesterics	129
B. Kamenar, M. Penavić, and A. Hergold-Brundić: The Crystal Structure of Phenylmercury(II) Trifluoroacetate and the Refinement of the Crystal Structure of Phenylmercury(II) Acetate	145
M. Lovrić, T. Magjer, and M. Branica: Electrochemical Kinetic Measurements and Metal Speciation with the Vibrating Dropping Mercury Electrode	153
K. Kovačević, Z. B. Maksić, and A. Moguš-Milanković: Geometry of Molecules. Part 7. Interatomic Distances, Bond Angles and Strain Energies in some Rotenes and Related Spirocompounds by the IMO Method	187
M. Cvetkovska, T. Grčev, and G. Petrov: Investigations Electrochimiques des Systèmes Rédox: Fe^{3+} , $\text{Fe}(\text{III})$ -Complexe, Cu^{2+} , $\text{Cu}(\text{II})$ -Complexe- <i>meta</i> -Bisulfite de Sodium, Initiateurs de Polymérisation de l'Acrylamide en Milieu Aqueous	201
M. F. Hussain, R. K. Bansal, and B. K. Puri: Solid-liquid Separation after Liquid-liquid Extraction: Spectrophotometric Determination of Cobalt by Extraction of its 2-Methoxyethyl Xanthate in Molten Naphthalene	219
T. M. Krygowski, T. Wieckowski, and A. Sokolowska: Infrared and Raman Studies of Carbonyl Group Frequencies of <i>p</i> -Substituted Benzoic Acids in the Crystalline State	229
R. Jain: Elucidation of the Structure of Some Potential Antidiabetic Pyrazolin-5-ones Using Polarographic Technique	235

B. S. Chandravanshi and V. K. Gupta: Extraction and Spectrophotometric Determination of Cerium(IV) with <i>N-p</i> -Chlorophenylcinnamohydroxamic Acid	243
M. Biruš, N. Kujundžić, M. Pribanić, and Z. Tabor: Equilibrium Studies on Complexation of Iron(III) by Acet-, Glycinium and Betaine Hydroxamic Acids	313
H. Vogler: Donor-Acceptor Cyclophanes with Biradical-Ionic Ground States	325
M. Ladika, D. E. Sunko, and S. Borčić: Solvolysis Rate of 3-Methyl-2-(3-pentynyl)-2-cyclohexenyl <i>p</i> -Nitrobenzoate. A Model System for π -Participation of the CC Triple Bond	331
S. El-Basil, P. Krivka, and N. Trinajstić: Application of the Dualist Model. Generation of Kekulé Structures and Resonant Sextets of Benzenoid Hydrocarbons	339
C. Carter and J. N. Murrell: Analytical Two-valued Potential Energy Functions for the Ground State Surfaces of $\text{CO}_2(\tilde{\text{X}}^1\Sigma_g^+)$ and $\text{CS}_2(\tilde{\text{X}}^1\Sigma_g^+)$	355
T. P. Živković: Splitting of the Configuration Interaction Space X_n into Two Complementary Subspaces	367
A. T. Balaban and I. Tomescu: Chemical Graphs. XL. Three Relations Between the Fibonacci Sequence and the Numbers of Kekulé Structures for Non-branched cata-Condensed Polycyclic Aromatic Hydrocarbons	391
N. Bresciani-Pahor, J. D. Orbell, and L. Randaccio: Steric Influences in Octahedral Cobaloximes. The Crystal and Molecular Structure of <i>trans</i> -methylbis(dimethylglyoximato)(phosphite)cobalt-(III) Complex with Phosphite= $\text{P}(\text{OMe})_2\text{Ph}$ and $\text{P}(\text{OMe})\text{Ph}_2$	433
M. J. Malinar, P. N. Radivojša, K. Marković, D. Belić, and M. B. Ćelap: Synthesis and Configuration of New Isomers of the Bis(aminocarboxylato)carbonatocobaltate(III) Ion	443
P. Radivojević, N. Milinski, B. Ribár, and D. Lazar: The Crystal Structure of the Complex $[\text{Y}(\text{H}_2\text{O})_5(\text{NO}_3)_2][\text{Y}(\text{H}_2\text{O})_2(\text{NO}_3)_4]$	451
E. C. Alyea, S. A. Dias, G. Ferguson, and P. Y. Siew: Structural Studies of Steric Effects in Phosphine Complexes. Part XII. Synthesis, Characterisation, and Crystal and Molecular Structure of Bis(trifluoroacetato)(trimesitylphosphine)mercury(II) Dimer, $[\text{Hg}(\text{CF}_3\text{CO}_2)_2\text{P}(\text{mesityl})_3]_2$	457
W. H. Watson and W. W. Holley: The Structure of Four Complexes of 2,2,6,6-Tetramethyl-3,5-heptanedione Containing One, Four, Four and Nine Cu(II) Ions	467
P. Bronzan-Planinić and H. Meider: Synthesis and Characterization of Cobalt(II), Nickel(II) and Copper(II) Chloride Complexes with Bis[(diphenylphosphinyl)methyl]phenylphosphine Oxide and Bis[(diphenylphosphinyl)methyl]-phosphinic Acid	477
G. B. Carpenter: The Conventional Bravais Unit Cell from Diffractometer Data	491
P. Engel and W. Nowacki: Refinement of the Crystal Structure of Synthetic Tl_3AsS_4	499
D. Doppelt, J. Fischer, and R. Weiss: Synthesis and Structure of a Dimercapto-Iron(III) Porphyrin Derivative: $[\text{Fe}(\text{SC}_6\text{HF}_4)_2\text{TPP}] \parallel \text{Na} \subset 18\text{C}_6 \parallel \text{C}_6\text{H}_6$	507
A. Kálmán, G. Argay, B. Ribár, S. Vladimirov, and D. Živanov-Stakić: Crystal and Molecular Structure of 3 β -Hydroxy-14,15 β -epoxy-5 β ,14 β -card-20,22-enolide (Digirezigenin)	519
N. Brničević, Š. Mesarić, and H. Schäfer: Cluster Hydroxides of the Composition $\text{M}_2[\text{Ta}_6\text{Cl}_{12}] (\text{OH})_6 \cdot n\text{H}_2\text{O}$, with $\text{M}=\text{Na, K, Rb, (CH}_3)_4\text{N}^+$; and $(\text{C}_2\text{H}_5)_4\text{N}^+$; Air Oxidation of the Cluster Unit $[\text{Ta}_6\text{Cl}_{12}]^{2+}$ in Alkaline Medium	529
B. Nowitzki and R. Hoppe: Eine Bemerkung über $\text{K}_2[\text{NiO}_2]$	537
L. P. Battaglia, A. Bonamartini Corradi, and M. Nardelli: Structural Aspects of 2-Thioimidazolidine Coordination in Silver(I) Halide Complexes	545

Lj. Golič, I. Leban, and P. Šegedin: Behaviour of Dimolybdenum Tetraacetate in Aqueous Solutions of Hydrogen Halides. Synthesis and Crystal Structures of $(pyH)_2[Mo_2(O_2CCH_3)_4Br_2]$ and two Modifications of $(pyH_2)[Mo_2(O_2CCH_3)_4I_2]$ (py =pyridine)	565
B. V. Prelesnik and R. M. Herak: The Crystal Structure of $trans(NO_2, N=C-CH_3)-(N\text{-ethylidene}\text{-ethylene}\text{-diamine})\text{-glycylglycinato}nitrocobalt(III)$ Monohydrate, $[Co(glygly)\text{---NO}_2(CH_3CH=en)]\cdot H_2O$	577
Lj. Manojlović-Muir and K. W. Muir: A Novel Pt(II)-Pt(IV) Mixed Valence Complex: The Crystal and Molecular Structure of $[LP(\mu-I)(\mu-Me_2PCH_2PMMe_2)_2]PtMe_3[I_3]$, $L=0.45I+0.55Me$	587
N. Galešić, B. Matković, M. Topić, E. Coffou, and M. Šljukić: The Crystal Structure of Disodium Thorium Biphosphate, $Na_2Th(PO_4)_2$	597
M. Hercog, B. Matković, D. Sevdic, D. Matković-Čalogović, and A. Nagl: A Folded Conformation of 1,4,8,11-Tetrathiacyclotetradecane in its Mercury Compound: $1,4,8,11\text{-Tetrathiacyclotetradecanedipicratomercury(II)}$ Heminitromethane, $[Hg(C_{10}H_{20}S_4)\cdot(C_6H_2N_3O_7)_2]\cdot 1/2CH_3NO_2$	609
I. Matijašić, G. D. Andreetti, P. Sgarabotto, A. Bezjak, and D. Fleš: Crystal and Molecular Structure of (S)- α -(p-Bromobenzenesulphonamido)- β -propiolactone	621
L. Colombo, G. Baranović, J. R. Durig, and A. E. Stanley: Polarized Infrared Spectra of Tolane Single Crystal	629
B. Kamenar, M. Penavić, and B. Marković: The Crystal Structure of Pyridinium μ -salicylato-tetrachloro- μ -oxo- μ -ethoxy-dioxodimolibdate(V)	637
T. Balić-Žunić, S. Šćavničar, and Z. Grobenski: The Structure of Thorium(IV) Dittitanium(IV) Oxide, $ThTi_2O_6$	645
A. E. Elia, E. C. Lingafelter, and V. Schomaker: The Crystal Structure of (2,3,9,10-tetramethyl-1,4,8,11-tetraaza-1,3,8,10-cyclotetradecatetraene)copper(II) Tetraphenylborate	653
B. Kojić-Prodić, Ž. Ružić-Toroš, G. Snatzke, and J. J. Herak: An Absolute Configuration of (1R, 4R, 5R)-4-Methoxy-8-acetyl-7,7-dimethyl-6-thia-3,8-diazabicyclo[3.2.1]octan-2-one, $C_{10}H_{16}N_2O_3S$	661
M. Pušelj, Z. Ban, and A. Szitula: The Crystal Structure and Magnetic Properties of the $Cu_2MnAl_{1-x}Hg_x$ System	669
A. Demšar and P. Bukovec: Synthesis and Crystal Structure of Tetraethylammonium Di- μ -fluoro-bis-[aquadifluoro-oxovanadate(IV)]	673
J.-P. Charland and A. L. Beauchamp: Crystal Structure and Infrared Spectra of Anhydrous (Adeninato)methylmercury(II)	679
B. Korpar-Čolig, Z. Popović, and M. Sikirica: Mercuration of Some Aliphatic Aldehydes. The Crystal Structure of 2,2-Bis(chloromercuri)butyraldehyde	689
M. A. Beno, R. Sundell, and J. M. Williams: The Hydrogendifluoride Anion in an Asymmetric Crystalline Environment: The Crystal and Molecular Structure of Trithioureatellurium(II) Di(Hydrogendifluoride)	695
L. G. Kuz'mina and Y. T. Struchkov: Structural Chemistry of Organomercury Compounds. Role of Secondary Interactions	701
A. L. Mackay: Descriptors for Complex Inorganic Structures	725
R. D. Willett and U. Geiser: Structural Characteristics of $ACuCl_3$ Salts	737
S. Popović: Application of Bell-Shaped Functions in X-ray Diffraction Broadening Analysis	749
G. B. Deacon, A. Florenti, M. Hughes, and F. P. Larkins: An Investigation of the Acceptor Properties of Some Organomercurials by Molecular Weight Measurements and X-ray Photoelectron Spectroscopy	757
Z. S. Herman and L. Pauling: Hybrid Bond Orbitals and Bond Strength for Pentacovalent Bonding	765
W. E. Palke: On Determining Orbital Hybridization	779
G. Del Re and C. Barbier: <i>In Situ</i> Atomic Orbitals and Extended Basis Molecular Calculations	787

D. Lj. Vučković and Lj. Vujisić: Structure and Properties of Small Ring Propellanes by the IMO Method	801
K. H. Aufderheide: A Localized Atomic Orbital Description of the Rotational Barrier in Ethane	811
P. R. Surján: The Representation of the Chemical Bond in Quantum Chemical Calculations	833
E. Kapuy, Z. Csépes, and C. Kozmutza: Many-Body Perturbation Theory Based on Localized Orbitals	855
R. McWeeny: Weak Interactions Between Molecules	865
A. Garcia-Leigh and J. N. Murrell: On the Stability of BH_3 and BF_3 Adducts with BF_3 , CO and N_2	879
M. Klessinger: Fragment Molecular Orbitals for Molecules and Interacting Systems	887
G. Náray-Szabó: Chemical Fragmentation for Molecular Orbital Calculations on Proteins	901
F. Bernardi, A. Bottini and G. Tonachini: A Quantitative Analysis of the Role of Non-Bonded and Geminal Interactions in $\text{H}_2\text{N}-\text{X}$ Molecules	911
L. S. Bartell: Do the VSEPR Points-on-a-Sphere Repulsions Simulate Quantum Interactions?	927
K. Jug: Bond Order as a Tool for Molecular Structure and Reactivity	941
B. M. Gimarc: Nonbonded Bond Orders, Molecular Conformations and Relative Stabilities of Sulfur-Nitrogen Rings and Chains	955
E. Honegger, Z.-Z. Yang, and E. Heilbronner: The Equivalent Bond Orbital Model Revisited: I. Orbitals, Orbital Energies and PE Spectra of Saturated Hydrocarbons	967
J. Spanget-Larsen: Breakdown of the One-Electron Picture of Ionization for Hydrocarbon π -Systems	991
J. E. Bloor and R. E. Sherod: An Overlapping Spheres Multiple Scattering χ_a Study of the Perfluoro Effect on the Ionization Potentials and Electron Transmission Spectra of Fluorosubstituted Benzenes	1011
N. D. Epotis, J. R. Larson, and H. H. Eaton: »Common Denominators« by the MOVB Method: The Structures of H_2O , H_2O_2 and their Derivatives	1031
P. Politzer and B. A. Zilles: Some Observations Concerning Electronic Densities, Electrostatic Potential and Chemical Potential	1055
D. Hadži, M. Hodošek, D. Kocjan, T. Šolmajer, and F. Avbelj: The Molecular Electrostatic Potential as a Determinant of Receptor-Drug Recognition	1065
M. Kibler: Symmetry Adaptation and Wigner-Racah Algebras in Quantum Chemistry	1075
C. J. Ballhausen: The $E \otimes \varepsilon$ Jahn-Teller Coupling: Models and Manifestations	1097
M. L. Ellzey, Jr.: Derivation of the AOM Parametrization from the Effective Hamiltonian for Complexed Transitional Metal Ions with Application to Effectively Tetragonal Four-Coordinate Systems	1107
M. Grodzicki: The Applicability of Point-Charge Approximations to the Calculations of Molecular Expectation Values	1125
B. Galabov, B. Nikolova, and W. J. Orville-Thomas: Infrared Band Intensities Electronic Charge Distribution in Molecules and Polar Properties of Valence Bonds	1145
R. C. Haddon and H. D. Roth: Homoconjugation in Radical Cations	1165
H. Vogler: A Theoretical Study of the ^1H -Chemical Shifts of $[4n]$ - and $[4n+2]$ Annulenes and their Di- and Tetraanions	1177
J. K. Burdett, S. Lee, and W. C. Sha: The Method of Moments and Energy Levels in Molecules and Solids	1193
N. Raos and Vl. Simeon: Conformational Analysis of Bis-(<i>N,N</i> -dimethyliso-leucinato)-Copper(II): Estimation of the Diastereoselectivity Effect by Means of two Approximate Methods	1217
A. Koukoulas and M. A. Whitehead: Penetration in the CNDO Theory	1225

C. Trindle: The Hierarchy of Models in Chemistry	1231
B. Kirtman and W. E. Palke: Factors Governing Nuclear Geometry and Bond-Orbital Directions in Second Row AH_3 Molecules	1247
D. Cremer and E. Kraka: A Description of the Chemical Bond in Terms of Local Properties of Electron Density and Energy	1259
W. L. Luken: Properties of the Fermi Hole in Molecules	1283
Z. B. Maksić, M. Eckert-Maksić, and K. Rupnik: Model Description of Some Molecular Properties by the Modified-Atom-in-a-Molecule (MAM) Approach	1295
S.-K. Kang, T. A. Albright, and J. Silvestre: The Bonding of P_4 to $d^8\text{-ML}_3$ Complexes	1355
H. Nakatsuji and M. Hada: Interaction of the Hydrogen Molecules with the Palladium Atom. A Force Theoretic Study	1371
E. Ortoleva and M. Simonetta: A Theoretical Study of the Influence of Surface Structure on Chemosorption of Nitrogen on Iron Single-Crystal Faces	1387
M. Persico and J. Tomasi: An Evaluation of Solvent Effects on Isomerization Mechanisms in Diimide and Methylenimine	1395
G. Klopman and M. R. Frierson: The Alpha-Efect. A Theoretical Study Incorporating Solvent Effect	1411
H. O. Villar, O. G. Stradella, R. E. Cachau, and E. A. Castro: Some Comments on the Nucleation Phenomena	1417
M. V. Basilevsky, N. N. Weinberg, and M. V. Zhulin: Where is the Limit to which the Qualitative Theory of Chemical Reactivity can be Extended? Study of Dienophilic Activity of Cyanoethylenes	1423
P. N. Skancke: A Molecular-Orbital Study of the Thermal Walk Rearrangement of Bicyclo[2.1.0]pent-2-ene	1445
W.-K. Ip and W.-K. Lee: MNDO Study of the Dimerization of Borane	1451
F. Volatron, Y. Jean, and Nguyêñ. T. Anh: The Role of Lone Pairs in Heteroatomic Chemistry. Graphical Analysis and <i>Ab Initio</i> Calculations of Oxirane and Aziridine Ring Opening	1461
J. B. Moffat: Partitioning and Additivity of the Chemical Bond	1475
C. Petrongolo: Non Adiabatic Effects and Radiationless Transitions	1485
A. Julg: The Problem of Enantiomers: Support for a New Interpretation of Quantum Mechanics	1497
M. Kibler and T. Négadi: On the Use of Nonbijective Canonical Transformations in Chemical Physics	1509
K. Balasubramanian: Recent Applications of Group Theoretical Generators to Chemical Physics	1525
T. P. Živković: The Splitting Theorem and Properties of Alternant Systems	1553
T. P. Živković: Antialternant Perturbations of Alternant Systems	1575
A. Graovac and O. E. Polansky: Topological Effect on Molecular Orbitals. Part 8. A Study of two Further Classes of Topologically Related Isomers	1595
L. v. Szentpály and W. C. Herndon: A Comparison of Pencil and Paper Procedures, PMO, Free Electron PMO, and Structure-Resonance Theory Calculations for Proton Affinities	1621
M. Grzonka, J. V. Knop, L. Klasinc, and N. Trinajstić: Theoretical Studies on Small Ring Heteropropellanes. Oxapropellanes	1629
T. Hirano and E. Ōsawa: On the Correspondence between Molecular Orbital Energies and Empirical Force Field Potential Terms	1633
V. Kvasnička: Second Quantization Formalism for Geminals	1643
V. Kellö, I. Hubač, A. I. Boldyrev, and V. Špirko: <i>Ab Initio</i> MBPT(4) Calculations of the Inversion Potential Function of NH_3	1661
E. W. Thulstrup: Interpretation of Optical Spectra of Partially Aligned Samples	1667

CHEMICAL SYNTHESIS

V. Šunjić, Š. Šimaga, and Lj. Vitale: The Synthesis and Angiotensin Converting Enzyme Inhibitory Activities of <i>N</i> -(3-Substituted)aminocarbonyl propanyl-L-prolines	251
V. Rapić and I. Habuš: Ferrocene Compounds. XII. Reactions of Ferrocene-carbaldehyde with Benzanilides and <i>n</i> -Butyllithium	265
S. Djokić, B. Gašpert, I. Lukić, Z. Mandić, B. Šimunić, M. Tomić, and A. G. Maasböl: <i>N</i> -4-Chlorobutyryl Aminoacids as a Common Intermediate in the Synthesis of <i>N</i> -Alkylamides of 2-Oxo-Pyrrolidine and L-Aspartyl-L-Phenylalanine Esters	271
M. V. Proštenik, M. Dumić, and I. Butula: Chemistry of 1,3-Dioxepins. II. Dehydrohalogenation of 5,6-Dihalogen-1,3-Dioxepanes with Strong Bases	281
M. Dumić, M. V. Proštenik, J. Fabijanić, und I. Butula: Chemie der 1,3-Dioxepine; III. Palladium-katalysierte Isomerisierung von 4,7- zu 6,7-Dihydro-1,3-dioxepinen	405

BIOCHEMISTRY

J. Kobe, Z. Crnjak Orel, and J. Kidrič: Complex Formation Between the Antiviral Nucleoside Ribavarin (1- β -D-Ribofuranosyl-1,2,4-Triazole-3-Carb oxamide) and Bivalent Metal Ions: ^1H and ^{13}C NMR Studies, and Comparison with Inosine	165
B. Mulac-Jeričević, B. Vranešić, S. Kveder, B. Jamnicky, and D. Keglević: Crystalline Suspension of Bovine Zinc Des-AlaB30-Insulin with Prolonged Hypoglycaemic Activity	289
J. Kobe, B. Rusjakovski, and B. Brdar: The Synthesis of Antiviral Activities of 2-Substituted Azino-3- β -D-ribofuranosyl and α and β -D-arabinofuranosyl-5-carbamoylmethylenethiazolidine-4-ones	295
D. Vasić-Rački: Immobilization of Yeast Alcohol Dehydrogenase on Weakly Basic Anion Exchange Resin Beads	305
Š. Škarić, M. Pavela-Vrančić, and J. Matulić-Adamić: Stereoselective Transformations in the Thymidine Series	415
J. Babnik, T. Lah, V. Cotić, and V. Turk: Anticathepsin D Antibody-Sepharose Chromatography of Human Cathepsin D	425

ANALYTICAL CHEMISTRY

V. Grdinić and M. Jakševac-Mikša: Microdetection of Some Biologically Active Thiol Compounds with Sodium Pentacyanoammineferrate(II) on Ion-Exchange Resin Grains	411
--	-----

PRELIMINARY COMMUNICATIONS

GENERAL AND THEORETICAL CHEMISTRY

M. Ladika and D. E. Sunko: Allylic Cations in Solvolysis. A Case of Non-Participation	179
--	-----

CHEMICAL SYNTHESIS

V. Škarić and Dj. Škarić: Novel Syntheses of Thiazolo[3,2-a]pyrimidin-7-ones	183
---	-----

SADRŽAJ

ORIGINALNI ZNANSTVENI RADOVI

OPĆA I TEORIJSKA KEMIJA

S. El-Basil: Jednostavan kombinatorni algoritam za konstrukciju sekstetnog polinoma kata-kondenziranih benzenoidnih ugljikovodika	1
S. El-Basil: Molekularna topologija i molekularna svojstva. I. Sekvencijske oznake kata-kondenziranih benzenoidnih ugljikovodika koji sadrže do pet prstenova	21
S. El-Basil: O graf-teorijskom pristupu Kekuléovim strukturama. Novi identiteti sekstetnih polinoma i veza s Clarovom teorijom seksteta	47
H. Hodošek, D. Kocjan in T. Šolmajer: Študij kompleksa noradrenalin-mravlja kiselina	65
M. Topić i A. Moguš-Milanković: Višestruka termička analiza amonij heptamolibdat tetrahidrata	75
A. Julg i B. Deprick: Teorijska studija adsorpcije karbonilnih spojeva na ionskim kristalima: I. Formaldehid, glioksal, o- i p-benzokinon na (100) plohi natrij klorida	85
D. Težak, F. Strajnar, O. Milat, M. Stubičar i D. Šarčević: Ravnoteže čvrsto/tekuće u vodenim sustavima dodecil benzen sulfonata i zemnoalkalijskih iona	93
S. K. Dua, V. Kapur i S. K. Sahni: Titanat(IV)-, cirkonil(IV)-, hafnil(IV)-, i uranil(VI)-kompleksi terdentatnih benzoilhidrazona	109
Lj. Tušek-Božić i B. Božić: Ispitivanje vodljivosti ionskih parova kompleksa nekih makrocikličkih polietera s pikratima i tetrafenilboratima alkalnih metala u metanolu	119
D. Dasić, M. E. Marcondes H., L. W. Reeves i M. Szarka: Micelarni oblici kod liotropnih nematičkih i kolesterolskih tekućih kristala	129
B. Kamenar, M. Penavić i A. Hergold-Brundić: Kristalna struktura fenilživa (II)-trifluoroacetata i utočnjavanje strukture fenilživa(II)-acetata	145
M. Lovrić, T. Magjer i M. Branica: Elektroanalitička primjenjivost živine elektrode koja vibrira	153
K. Kovačević, Z. B. Maksić i A. Moguš-Milanković: Geometrija molekula. 7. Međuatomske udaljenosti, kutevi između veza i energije napetosti kod nekih rotena i sličnih spiro spojeva studiranih IMOAA metodom	187
M. Cvetkovska, T. Grčev i G. Petrov: Elektrohemijska ispitivanja redoks sistema: Fe^{3+} , $\text{Fe}(\text{III})$ -kompleksi, Cu^{2+} , $\text{Cu}(\text{II})$ -kompleksi — $\text{Na}_2\text{S}_2\text{O}_5$, za iniciranje polimerizacije akrilamida u vodenoj sredini	201
M. F. Hussain, R. K. Bansal i B. K. Puri: Spektrofotometrijsko određivanje kobalt-2-metoksietil-ksantata nakon njegove ekstrakcije u rastaljenom naftalenu i separacije čvrste i tekuće faze	219
T. M. Krygowski, T. Wieckowski i A. Sokolowska: Frekvencije karbonilne grupe u infracrvenim i Raman spektrima za <i>p</i> -supstituirane benzojeve kiseline u kristalnom stanju	229
R. Jain: Određivanje strukture nekih potencijalnih antidiabetskih pirazolin-5-iona pomoću polarografske metode	235
B. S. Chandravanshi i V. K. Gupta: Ekstrakcija i spektrofotometrijsko određivanje cera(IV) s <i>N-p</i> -klorofenilcinamohidroksamatom kiselinom	243

M. Biruš, N. Kujundžić, M. Pribanić i Z. Tabor: Istraživanje ravnoteže pri kompleksiranju željezo(III)-iona s acet-, glicinium i betain-hidroksamatom kiselinama	313
H. Vogler: Donor-akceptorski ciklofani s biradikalno-ionskim osnovnim stanjima	325
M. Ladika, S. Borčić i D. E. Sunko: Brzina solvolize 3-metil-2-(3-pentinil)-2-cikloheksenil-p-nitrobenzoata. Modelni sistem za π -participaciju trostrukre veze CC	331
S. El-Basil, P. Krivka i N. Trinajstić: Primjena dualističkog modela. Generiranje Kekuléovih struktura i rezonancijskih seksteta benzoidnih ugljikovodika	339
S. Carter i J. N. Murrell: Analitičke dvovrijednosne potencijalne energijske funkcije za površine temeljnog stanja od $\text{CO}_2(\tilde{\text{X}}^1\Sigma_g^+)$ i $\text{CS}_2(\tilde{\text{X}}^1\Sigma_g^+)$	355
T. P. Živković: Cijepanje konfiguracijsko-interakcijskog prostora X_n na dva komplementarna podprostora	367
A. T. Balaban i I. Tomescu: Kemijski grafovi. 40. Tri relacije između Fibonacijevog niza i brojeva Kekuléovih struktura za nerazgranate katakondenzirane polickličke aromatske ugljikovodike	391
N. Bresciani-Pahor, J. D. Orbell i L. Randaccio: Sterički utjecaji u oktaedarskom kobaloksimima. Kristalna i molekulska struktura <i>trans</i> -metilbis(dimetilglioksimato(fosfit)kobalt(III) kompleksa s fosfit = $\text{P}(\text{OMe})_2\text{Ph}$ i $\text{P}(\text{OMe})\text{Ph}_2$)	433
M. J. Malinar, P. N. Radivojša, K. Marković, D. Belić i M. B. Ćelap: Sinteza i konfiguracija novih izomera bis(amino-karboksilato)-karbonato-kobalt (III) iona	443
P. Radivojević, N. Milinski, B. Ribár i D. Lazar: Kristalna struktura kompleksa $[\text{Y}(\text{H}_2\text{O})_5(\text{NO}_3)_4] \cdot [\text{Y}(\text{H}_2\text{O})_2(\text{NO}_3)_2]$	451
E. C. Alyea, S. A. Dias, G. Ferguson i P. Y. Siew: Strukturno proučavanje steričkih efekata u fosfinskim kompleksima. Dio XII. Sinteza, karakterizacija, te kristalna i molekularna struktura bis(trifluoroacetato)trimetilfosfin-živa(II)-dimeru $[\text{Hg}(\text{CF}_3\text{CO}_2)_2\text{P}(\text{mezitil})_3]^2+$	457
W. H. Watson i W. W. Holley: Strukture četiri 2,2,6,6-tetrametil-3,5-heptan-dionova kompleksa s jednim četiri, četiri i devet Cu(II) iona	467
P. Bronzan-Planinić i H. Meider: Priprava i opis kompleksa kobalt(III)-nikal (II)- i bakar(II)-klorida s bis[(difenilfosfinil)metil]fenilfosfin oksidom i bis[(difenilfosfinil)metil]-fosfinskom kiselinom	477
G. B. Carpenter: Konvencionalna Bravaisova jedinična celija iz difraktometrijskih podataka	491
P. Engel i W. Nowacki: Utočnjavanje kristalne strukture sintetskog Tl_3AsS_4	499
P. Doppelt, J. Fischer, R. Weiss: Sinteza i struktura jednog dimerkapto-željezo (III) porfirinskog derivata: $[\text{Fe}(\text{SC}_6\text{HF}_4)_2\text{TPP}] \cdot \text{NaCl} \cdot 18\text{C}_6 \cdot \text{C}_6\text{H}_6$	507
A. Kálmán, G. Argay, B. Ribár, S. Vladimirov i D. Živanov-Stakić: Kristalna i molekulska struktura 3β -hidroksi-14,15 β -epoksi-5 β ,14 β -kard-20,22-enolida (Digirezigenin)	519
N. Brničević, Š. Mesarić i H. Schäfer: Klasterski hidroksidi sastava $\text{M}_2[\text{Ta}_6\text{Cl}_{12}](\text{OH})_6 \cdot n\text{H}_2\text{O}$, $\text{M}=\text{Na, K, Rb, (CH}_3)_4\text{N}^+$; Oksidacija klasterske jedinice $[\text{Ta}_6\text{Cl}_{12}]^{2-}$ kisikom iz zraka u lužnatom mediju	529
B. Nowitzki i R. Hoppe: Neka zapažanja o $\text{K}_2[\text{NiO}_2]$	537
L. P. Battaglia, A. Bonamartini Corradi i I. M. Nardelli: Strukturni aspekti 2-tioimidazolidin koordinacije u srebro(I) halidnim kompleksima	545
Lj. Golić, I. Leban in P. Šegedin: Obnašanje dimolibdenovega tetraacetata v vodnih raztopinah vodikovih halogenidov. Sinteze in kristalne strukture $(\text{pyH})_2[\text{Mo}_2(\text{O}_2\text{CCH}_3)_4\text{Br}_2]$ in dveh modifikacij $(\text{pyH})_2[\text{Mo}_2(\text{O}_2\text{CCH}_3)_4\text{I}_2]$ (py =piridin)	565
B. V. Prelesnik i R. M. Herak: Kristalna struktura $trans(\text{NO}_2, \text{N}=\text{C}-\text{CH}_3)-(\text{N}-\text{etiliiden-etenil-diamin})-(\text{glicil-glicinato})-\text{nitro-kobalt(III)}\text{monohidrata, } [\text{Co}(\text{glygly})\text{NO}_2(\text{CH}_3\text{CH=en})] \cdot \text{H}_2\text{O}$	577

Lj. Manojlović-Muir i K. W. Muir: Novi Pt(II)–Pt(IV) kompleks miješane valencije: Kristalna i molekulska struktura [LP(μ -I) (μ -Me ₂ PCH ₂ PM ₂) ₂ PtMe ₃]I ₃ , L = 0,45I + 0,55Me	587
N. Galešić, B. Matković, M. Šljukić, M. Topić i E. Coffou: Kristalna struktura dinatrijtorijevog bifosfata, Na ₂ Th(PO ₄) ₂	597
M. Herceg, B. Matković, D. Sevdic, D. Matković-Čalogović i A. Nagl: Svinuta konformacija 1,4,8,11-tetratriciklotetradekana u živinu spoju 1,4,8,11-te-tratriciklotetradekandipikratoživa(II)-heminitrometan, [Hg(C ₁₀ H ₂₀ S ₄)·(C ₆ H ₂ N ₃ O ₇) ₂]·1/2 CH ₃ NO ₂	609
I. Matijašić, G. D. Andreetti, P. Sgabarro, A. Bezjak i D. Fleš: Kristalna i molekularna struktura (S)(<i>p</i> -bromobenzensulfonamido- β -propiotiolaktona)	621
L. Colombo, G. Baranović, J. R. Durig i A. E. Stanley: Spektri tolana	629
B. Kamenar, M. Penavić i B. Marković: Kristalna struktura piridinij- μ -sali-cilato-tetrakloro- μ -okso- μ -etoksodioksodimolibdata(V)	637
T. Balić Žunić, S. Šćavničar i Z. Grobenski: Struktura ThTi ₂ O ₆	645
A. E. Elia, E. C. Lingafelter i V. Schomaker: Kristalna struktura (2,3,9,10-tetra-metil-1,4,8,11-tetraaza-1,3,8,10-ciklotetradekatetraen)bakar(II)-tetrafenil-borata	653
B. Kojić-Prodić, Ž. Ružić-Toroš, G. Snatzke i J. J. Herak: Apsolutna konfiguracija (1R, 4R, 5R)-4-metoksi-8-acetyl-7,7-dimetil-tio-3,8-diazabiciklo[3.2.1]-oktan-2-ona, C ₁₀ H ₁₆ N ₂ O ₃ S	661
M. Pušelj, Z. Ban i A. Szitula: Kristalna struktura i magnetska svojstva sistema Cu ₂ MnAl _{1-x} Hg	669
A. Demšar i P. Bukovec: Sinteza in kristalna struktura tetraetilamonijevega di- μ -fluoro-bis[akovadifluorooxovanadat(IV)]	673
J.-P. Charland i A. L. Beauchamp: Kristalna struktura i infracrveni spektri bezvodne (adeninato)methylžive(II)	679
B. Korpar-Čolig, Z. Popović i M. Sikirica: Merkuriranje nekih alifatskih aldehida. Kristalna struktura 2,2-bis(kloromerkuri)butiraldehida	689
M. A. Beno, R. Sundell i J. M. Williams: Anion vodikovog diflorida u asimetričnom kristalnom okruženju: kristalna i molekularna struktura tritio-ureatetur(II) di(hidrogendiflorida)	695
L. G. Kuz'mina i Y. T. Struchkov: Strukturna kemija organoživinih spojeva. Uloga sekundarnih interakcija	701
A. L. Mackay: Deskriptori za kompleksne anorganske strukture	725
R. D. Willett i U. Geiser: Strukturne karakteristike ACuCl ₃ soli	737
S. Popović: Primjena zvonolikih funkcija u analizi rendgenskoga difrakcijskog proširenja	749
G. B. Deacon, A. Florenti, M. Hughes i F. Larkins: Istraživanje akceptorskih svojstava nekih organomerkurijala mjeranjem molekulske težine i rendgenskom fotoelektronском spektroskopijom	757
Z. S. Herman i L. Pauling: Hbridne orbitale i jačina pentakovalentnog vezanja	765
W. E. Palke: O određivanju hibridizacije orbitala	779
G. Del Re i C. Barbier: Atomske orbitale <i>in situ</i> i molekularni računi s proširenim skupovima osnovnih funkcija	787
D. Lj. Vučković i Lj. Vujišić: Strukturni parametri i svojstva malih propelana dobiveni primjenom IMO metode	801
K. H. Aufderheide: Opis rotacijske barijere etana s pomoću lokaliziranih atomskih orbitala	811
P. R. Surján: Opis kemijske veze u kvantnoj kemiji	833
E. Kapuy, Z. Csépés i C. Kozmutza: Perturbacijska teorija više tijela uporabom lokaliziranih orbitala	855
R. McWeeny: Slabe interakcije između molekula	865
A. Garcia-Leigh i J. N. Murrell: O stabilnosti adukata BH ₃ i BF ₃ s dvoatom-skim molekulama BF, CO i N ₂	879

M. Klessinger: Opis molekula i njihovih međudjelovanja s pomoću molekulskih orbitala njihovih fragmenata	887
G. Náray-Szabó: Molekulsko-orbitalni računi na proteinima primjenom postupka kemijske fragmentacije	901
F. Bernardi, A. Bottini i G. Tonachini: Kvantitativna analiza uloge neveznih i geminalnih interakcija kod molekula $\text{H}_2\text{N}-\text{X}$	911
L. S. Bartell: Da li odbijanje VSEPR »točaka-na-kugli« simulira kvantne interakcije?	927
K. Jug: Red veze kao pribor za proučavanje molekulskih struktura i reaktivnosti	941
B. M. Gimarc: Nevezni redovi veza, konformacije molekula i relativne stabilitosti $\text{S}-\text{N}$ prstena i lanaca	955
E. Honegger, Z.-z. Yang i E. Heilbronner: Preispitivanje modela ekvivalentnih veznih orbitala: I. Orbitalne, orbitalne energije i PE spektri zasićenih ugljikovodika	967
J. Spanget-Larsen: Slom jednoelektronske orbitalne slike kod ionizacije π -elektronskih ugljikovodika	991
J. E. Bloor i R. E. Sherrod: Studij utjecaja perfluoroefekta na ionizacijske potencijale i elektronske transmisione spektre fluorsupstituiranih benzene s pomoću $\text{X}\alpha$ -metode višestrukog raspršenja u aproksimaciji prekrivanja atomskih kugli (OSMS- $\text{X}\alpha$)	1011
N. D. Epotis, J. R. Larsen i H. H. Eaton: Metoda »zajedničkih nazivnika« s pomoću MOVB pristupa: Struktura molekula H_2O , H_2O_2 i njihovih derivata	1031
P. Politzer i B. A. Zilles: Neka zapažanja u vezi elektronskih gustoća, elektrostatskih potencijala i kemijskih potencijala	1055
D. Hadži, M. Hođošek, D. Kocjan, T. Šolmajer i F. Avbelj: Molekulski elektrostatski potencijal kao odlučujući faktor u određivanju prepoznavanja receptora i lijeka	1065
M. Kibler: Simetrijska adaptacija i Wigner-Racahove algebre u kvantnoj kemiji	1075
C. J. Ballhausen: $E \otimes \epsilon$ Jahn-Tellerovo sprezanje: Modeli i manifestacije	1097
M. L. Ellzey, Jr.: Izvod AOM parametrizacije iz efektivnog hamiltonijana za komplekse iona prijelaznih metala s primjenom na tetragonalne sustave koordinacije četiri	1107
M. Grodzicki: Primjenljivost aproksimacije točkastog naboja pri računanju očekivanih vrijednosti za molekule	1125
B. Galabov, B. Nikolova i W. J. Orville-Thomas: Intenziteti infracrvenih vrpcu, raspodjela naboja u molekulama i polarna svojstva kovalentnih veza	1145
R. C. Haddon i H. D. Roth: Homokonjugacija kod radikal-kationskih sustava	1165
H. Vogler: Teorijski studij kemijskih pomaka protona kod $[4n]$ - i $[4n+2]$ -anulena i njihovih di- i tetraaniona	1177
J. K. Burdett, S. Lee i W. C. Sha: Metoda momenata i energijske razine molekula i čvrstih tijela	1193
N. Raos i Vl. Simeon: Konformacijska analiza kompleksa bis-(N,N -dimetil-isoleucinato)-Cu(II): određivanje dijastereoselektivnog efekta s pomoću dvije aproksimativne metode	1217
A. Koukoulas i M. A. Whitehead: Integralni prodiranja u CNDO teoriji	1225
C. Trindle: Higerarhija modela u kemiji	1231
B. Kirtman i W. E. Palke: O faktorima koji određuju geometrijske rasporede jezgri molekula AH_2 i smjerove lokaliziranih veznih orbitala	1247
D. Cremer i E. Kraka: Opis kemijske veze s pomoću lokalnih svojstava elektronske gustoće i energije	1259
W. L. Luken: Svojstva Fermijeve šupljine u molekulama	1283
Z. B. Maksić, M. Eckert-Maksić i K. Rupnik: Opis molekulskih svojstava pomoću modela modificiranih atoma (MAM)	1295
S.-K. Kang, T. A. Albright i J. Silvestre: Vezanje P_4 na $\text{d}^8\text{-ML}_3$ kompleksima	1355

H. Nakatsuji i M. Hada: Interakcija molekule H_2 s atomom paladija primjenom koncepta Hellman-Feynmanove sile	1371
E. Ortoleva i M. Simonetta: Teorijsko razmatranje utjecaja strukture površina na kemosorpciju dušika na monokristale atoma željeza	1387
M. Persico i J. Tomasi: Procjena utjecaja otapala na mehanizme izomerizacije diimida i metilenimina	1395
G. Klopman i M. R. Frierson: Alfa-efekt. Teorijski studij s pomoću MINDO/3 metode i teorije solvatacije	1411
H. O. Villar, O. R. Stradella, R. E. Cachau i E. A. Castro: O pojavi nukleacije molekula	1417
M. V. Basilevsky, N. N. Weinberg i V. M. Zhulin: Do koje se granice može proširiti kvalitativna teorija kemijske reaktivnosti? Studij dienofilne aktivnosti cijanoetilena	1423
P. N. Skancke: Teorijski MO studij preuređenja biciklo[2.1.0]pent-2-ena putem termičkog koraka	1445
W.-K. Ip i W.-K. Li: Studij dimerizacije borana s pomoću MNDO metode	1451
F. Volatron, Y. Jean i Nguyén T. Anh: Uloga osamljenih parova kod heteroatomskih molekula. Analiza otvaranja oksiranskih i aziridinskih prstena s pomoću <i>ab initio</i> računa i grafova prekrivanja	1461
J. B. Moffat: Particija i aditivnost kemijske veze	1475
C. Petrongolo: Neadijabatski efekti i prijelazi bez zračenja	1485
A. Julg: Problem enantiomera: Potpora za novu interpretaciju kvantne mehanike	1497
M. Kibler i T. Négadi: Primjena nonbijektivnih kanonskih transformacija u kemijskoj fizici	1509
K. Balasubramanian: Neke primjene teorije grupa u kemijskoj fizici	1525
T. P. Živković: Teorem cijepanja i svojstva alternantnih sistema	1553
T. P. Živković: Antialternantne perturbacije alternantnih sistema	1575
A. Graovac i O. E. Polansky: Topološki efekt na molekularne orbitale. Dio 8. Studij dviju dalnjih klasa topološki vezanih izomera	1595
L. v. Szentpály i W. C. Herndon: Protonski afiniteti elektronskih molekula. Usporedba rezultata dobivenih s pomoću metoda PMO, FE-PMO i SR	1621
M. Grzonka, J. V. Knop, L. Klasinc i N. Trinajstić: Teorijski studij molekula heteropropelana. Oksapropelani	1629
T. Hirano i E. Ōsawa: O povezanosti energija molekulskih orbitala i članova empirijskoga potencijalnog polja	1633
V. Kvasnička: Formalizam druge kvantizacije za spregnute antisimetrične dvočestične valne funkcije (geminals)	1643
V. Kellö, I. Hubač, A. I. Boldyrev i V. Špirko: <i>Ab initio</i> MBPT(4) računi potencijala inverzije NH_3 molekule	1661
E. W. Thulstrup: Interpretacija optičkih spektara djelomično uređenih uzoraka	1667

KEMIJSKA SINTEZA

V. Šunjić, Š. Šimaga i Lj. Vitale: Sinteza derivata <i>N</i> -[(3-supstituiranih)amino-karbonil]propanoil-L-prolina i njihovo djelovanje na enzim za pretvorbu angiotenzina	251
V. Rapić i I. Habuš: Reakcije ferocenkarbaldehida, benzanilida i <i>n</i> -butil-litija	265
S. Djokić, B. Gašpert, I. Lukić, Z. Mandić, B. Šimunić, M. Tomić i A. G. Maasböl: <i>N</i> -4-klorbutiril aminokiseline kao intermedijeri u sintezi <i>N</i> -alkilamida 2-oxo-pirolidina i estera-L-fenilalanina	271
M. V. Proštenik, M. Dumić i I. Butula: Kemija 1,3-dioksepina. II. Dehidrohalogeniranje 5,6-dihalogen-1,3-dioksepana s jakim bazama	281
M. Dumić, M. V. Proštenik, J. Fabijanić i I. Butula: Kemija 1,3-dioksepina. III. Izomerizacija 4,7- u 6,7-dihidro-dioksepine na katalizatorima paladija	405

BIOKEMIJA

J. Kobe, Z. Crnjak Orel i J. Kidrič: Kompleksi antivirusnega nukleozida ribavrina (1β -D-ribofuranozil-1,2,4-triazol-3-karboksamid) z dvovalentnimi kovinskimi ioni: ^1H in ^{13}C NMR studja in primjerava z inozinom	165
B. Mulac-Jerićević, B. Vranešić, S. Kveder, B. Jamnický i D. Keglević: Kristalna suspenzija govedeg cink des-Ala-B30-insulina sa produženom hipoglikemičkom aktivnošću	289
J. Kobe, B. Rusjakovski in B. Brdar: Sinteza in antivirusna aktivnost 2-substituiranih azino- β -D-ribofuranozil in α in β -D-arabinofuranozil-5-karbamoilmetylentiazolidin-4-onov	295
D. Vasić-Rački: Imobilizacija alkoholne dihidrogenaze kvasca na slabobazičan anionski izmjenjivač	305
V. Škarić, M. Pavela-Vrančić i J. Matulić-Adamić: Stereoselektivne transformacije timidina	415
J. Babnik, T. Lah, C. Cotič i V. Turk: Immunoafinitetna kromatografija humana katepsina D	425

ANALITIČKA KEMIJA

V. Grdinić i M. Pakševac-Mikša: Mikrodokazivanje nekih bioloških aktivnih tiola s natrij-pentacijanoaminoferatom(II) na zrncima ionsko-izmjenjivačke smole	411
---	-----

PRETHODNA SAOPĆENJA

OPĆA I TEORIJSKA KEMIJA

M. Ladika i D. E. Sunko: Alilni kationi u solvolizi. Primjer izostanka partipacije	179
---	-----

KEMIJSKA SINTEZA

V. Škarić i D. Škarić: Nova sinteza tiazolo[3,2-a]pirimidin-7-ona	183
--	-----

INDEX

AUTORSKI INDEKS — AUTHORS INDEX

ORIGINALNI ZNANSTVENI RADOVI (OP) — ORIGINAL SCIENTIFIC PAPERS (OP)
BILJEŠKE (N) — NOTES (N)PRETHODNA SAOPĆENJA (PC) — PREMILINARY COMMUNICATIONS (PC)
PREDAVANJA (P) — CONFERENCE PAPER (P)**Albright, A.**: vidi **Kang, S.-K.****Alyea, E. C.**, **Dias, S. A.**, **Ferguson, G.** and **Siew, P. Y.**: Structural Studies of Steric Effects in Phosphine Complexes. Part XII. Synthesis, Characterization, and Crystal and Molecular Structure of Bis(trifluoroacetato)(trimesitylphosphine)mercury(II) Dimer, $[Hg(CF_3CO_2)_2P-(mesityl)_3]_2$ (OP)

457

Andreotti, G. D.: vidi **Matijašić, I.****Anh, Nguyêñ, T.**: vidi **Volatron, F.****Argay, G.**: vidi **Kálmán, A.****Aufderheide, K. H.**: A Localized Atomic Orbital Description of the Rotational Barrier in Ethane (OP)

811

Avbelj, F.: vidi **Hadži, D.****Babnik, J.**, **Lah, T.**, **Cotič, V.** and **Turk, V.**: Anticathepsin D Antibody-Sepharose Chromatography of Human Cathepsin D (OP)

425

Balaban, A. T. and **Tomescu, I.**: Chemical Graphs. XL. Three Relations Between the Fibonacci Sequence and the Numbers of Kekulé Structures for Non-branched cata-Condensed Polycyclic Aromatic Hydrocarbons (OP)

391

Balasubramanian, K.: Recent Applications of Group Theoretical Generators to Chemical Physics (OP)

1525

Balić Žunić, T., **Šćavničar, S.** and **Grobenski, Z.**: The Structure of Thorium (IV) Dititanium(IV) Oxide, $ThTi_2O_6$ (OP)

645

Ballhausen, C. J.: The $E \otimes \varepsilon$ Jahn-Teller Coupling: Models and Manifestations (AR)

1097

Ban, Z.: vidi **Pušelj, M.****Bansal, R. K.**: vidi **Hussain, M. F.****Baranović, G.**: vidi **Colombo, L.****Barbier, C.**: vidi **Del Re, G.****Bartell, L. S.**: Do the VSEPR Points-on-a-Sphere Repulsions Simulate Quantum Interactions? (OP)

927

Basilevsky, M. V., **Weinberg, N. N.** and **Zhulin, V. M.**: Where is the Limit to which the Qualitative Theory of Chemical Reactivity can be Extended? Study of Dienophilic Acitivity of Cyanoethylenes (OP)

1423

Battaglia, L. P., **Bonamartini Corradi, A.** and **Nardeli, M.**: Structural Aspects of 2-Thioimidazolidine Coordination in Silver(I) Halide Complexes (OP)

545

Beauchamp, A. L.: vidi **Charland, J.-P.****Belić, D.**: vidi **Malinar, K. J.****Beno, M. A.**, **Sundell, R.** and **Williams, J. M.**: The Hydrogendifluoride Anion in an Asymmetric Crystalline Environment: The Crystal and Molecular Structure of Trithioureatellurium(II) Di(Hydrogendifluoride) (OP)

695

Bernardi, F., **Bottone, A.** and **Tonachini, G.**: A Quantitative Analysis of the Role of Non-Bonded and Geminal Interactions in H_2N-X Molecules (OP)

911

Bezjak, A. : vidi Matijašić, I.	
Biruš, M., Kujundžić, N., Pribanić, M. and Tabor, Z. : Equilibrium Studies on Complexation of Iron(III) ba Acet-, Glycerinum and Betaine Hydroxamic Acids (OP)	313
Bloor, J. E. and Sherrod, R. E. : An Overlapping Spheres Multiple Scattering X α Study of the Perfluoro Effect on the Ionization Potentials and Electron Transmission Spectra of Fluorosubstituted Benzenes (OP)	1011
Boldyrev, A. I. : vidi Kellö, V.	
Bonamartini Corradi, A. : vidi Battaglia, L. P.	
Borčić, S. : vidi Ladika, M.	
Bottoni, A. : vidi Bernardi, F.	
Božić, B. : vidi Tušek-Božić, Lj.	
Branica, M. : vidi Lovrić, M.	
Brdar, B. : vidi Kobe, J.	
Bresciani-Pahor, N., Orbell, J. D. and Randaccio, L. : Steric Influences in Octahedral Cobaloximes. The Crystal and Molecular Structure of <i>trans</i> -methylbis(dimethylglyoximato)(phosphite)cobalt-(III) Complex with Phosphite = P(OMe) ₂ Ph and P(OMe)Ph ₂ (OP)	433
Brničević, N., Mesarić, Š., Schäfer, H. : Cluster Hydroxides of the Composition M ₂ [Ta ₆ Cl ₁₂](OH) ₆ ·nH ₂ O, with M=Na, K, Rb, (CH ₃) ₄ N ⁺ and (C ₂ H ₅) ₄ N ⁺ ; Air Oxidation of the Cluster Unit [Ta ₆ Cl ₁₂] ²⁺ in Alkaline Medium (OP)	529
Bronzan-Planinić, P. and Meider, H. : Synthesis and Characterization of Cobalt(II), Nickel(II), and Copper(II) Chloride Complexes with Bis[(diphenylphosphinyl)methyl]phenylphosphine Oxide and Bis[(diphenylphosphinyl)methyl]-phosphinic Acid (OP)	477
Bukovec, P. : vidi Demšar, A.	
Burdett, J. K., Lee, S. and Sha, W. C. : The Method of Moments and Energy Levels in Molecules and Solids (OP)	1193
Butula, I. : vidi Proštenik, M. V., Dumić, M.	
Cachau, R. E. : vidi Villar, H. O.	
Carpenter, G. B. : The Conventional Bravais Unit Cell from Diffractometer Data (OP)	491
Carter, C. and Murrell, J. N. : Analytical Two-valued Potential Energy Functions for the Ground State Surfaces of CO ₂ ($\tilde{\Sigma}^1 \Sigma_g^+$) and CS ₂ ($\tilde{\chi}^1 \Sigma_g$) (OP)	355
Castro, E. A. : vidi Villar, H. O.	
Chandravanshi, B. S. and Gupta, V. K. : Extraction and Spectrophotometric Determination of Cerium(IV) with <i>N</i> -p-Chlorophenylcinnamohydroxamic Acid (OP)	243
Charland, J.-P. and Beauchamp, A. L. : Crystal Structure and Infrared Spectra of Anhydrous (Adeninato)methylmercury(II) (OP)	679
Coffou, E. : vidi Galešić, N.	
Colombo, L., Baranović, G., Durig, J. R. and Stanley, A. E. : Polarized Infrared Spectra of Tolane Single Crystal (OP)	629
Cotić, V. : vidi Babnik, J.	
Cremer, D. and Kraka, E. : A Description of the Chemical Bond in Terms of Local Properties of Electron Density and Energy (OP)	1259
Crnjak Orel, Z. : vidi Kobe, J.	
Csépes, Z. : vidi Kapuy, E.	
Cvetković, M., Grčev, T. and Petrov, G. : Investigations Electrochimiques des Systèmes Rédox: Fe ³⁺ , Fe(III)-Complexe, Cu ²⁺ , Cu(II)-Complexe- <i>meta</i> -Bisulfite de Sodium, Initiateurs de Polymérisation de l'Acrylamide en Milieu Aqueux (OP)	201

Celap , M. B.: vidi Malinar , M. J.	
Deacon , G. B., Florenti , A., Hughes , M. and Larkins , F. P.: An Investigation of the Acceptor Properteis of Some Organomercurials by Molecular Weight Measurements and X-ray Photoelectron Spectroscopy (OP)	757
Del Re , G. and Barbier , C.: <i>In Situ</i> Atomic Orbitals and Extended Basis Molecular Calculations (OP)	787
Demšar , A. and Bukovec , P.: Synthesis and Crystal Structure of Tetraethyl-ammonium Di- μ -fluoro-bis-[aquadifluoro-oxovanadate(IV)] (OP)	673
Deprick , B.: vidi Julg , A.	
Dias , S. A.: vidi Alyea , E. C.	
Doppelt , P., Fischer , J. and Weiss , R.: Synthesis and Structure of a Dimer-campto-Iron(III) Porphyrin Derivative: $[\text{Fe}(\text{SC}_6\text{HF}_4)\text{TPP}] \parallel \text{Na} \subset 18\text{C}_6$, C_6H_6 (OP)	507
Dua , S. K., Kapur , V. and Sahni , S. K.: Titanyl(IV), Zirconyl(IV), Hafnyl(IV) and Uranyl(VI) Complexes of Terdentate Benzoyl Hydrazones (OP)	109
Dumić , M., Proštenik , M. V., Fabijanić , J. und Butula , I.: Chemie der 1,3-Dioxepine. III. Palladium-katalysierte Isomerisierung von 4,7- zu 6,7-Dihydro-1,3-dioxepine (OP)	405
Dumić , M.: vidi Proštenik , M. V.	
Durig , J. R.: vidi Colombo , L.	
Djokić , S., Gašpert , B., Lukić , I., Mandić , Z., Šimunić , B., Tomić , T. and Maasböl , A. G.: <i>N</i> -4-Chlorobutyryl Aminoacids as a Common Intermediate in the Synthesis o <i>N</i> -Alkylamides of 2-Oxo-Pyrrolidine and <i>L</i> -Aspartyl- <i>L</i> -Phenylalanine Esters (OP)	271
Eaton , H. H.: vidi Epiotis , N. D.	
Eckert-Maksić , M.: vidi Maksić , Z. B.	
El-Basil , S.: An Easy Combinatorial Algorithm for the Construction of Sextet Polynomials of Cata-condensed Benzenoid Hydrocarbons (OP)	1
El-Basil , S.: Molecular Topology and Molecular Properties I. »Sequence« Labels of Cata-condensed Benzenoid Hydrocarbons Containing up to Five Rings (OP)	21
El-Basil , S.: On a Graph-Theoretical Approach to Kekulé Structures. Novel Identities of Sextet Polynomials and a Relation to Clar's Sextet Theory (OP)	47
El-Basil , S., Krivka , P. and Trinajstić , N.: Application of the Dualist Model. Generation of Kekulé Structures and Resonant Sextets of Benzenoid Hydrocarbons (OP)	339
Elia , A. E., Lingafelter , E. C. and Schomaker , V.: The Crystal Structure of (2,3,9,10-tetramethyl-1,4,8,11-tetraaza-1,3,8,10-cyclotetradecatetraene) copper(II) Tetraphenylborate (OP)	653
Ellzey , Jr., M. L.: Derivation of the AOM Parametrization from the Effective Hamiltonian for Complexed Transitional Metal Ions with Application to Effectively Tetragonal Four-Coordinate Systems (OP)	1107
Engel , P. and Nowacki , W.: Refinement of the Crystal Structure of Synthetic Tl_3AsS_4 (OP)	499
Epiotis , N. D., Larson , J. R. and Eaton , H. H.: »Common Denominators« by the MOVB Method: The Structures of H_2O , H_2O_2 and their Derivatives (OP)	1031
Fabijanić , J.: vidi Dumić , M.	
Ferguson , G.: vidi Alyea , E. C.	
Fischer , J.: vidi Doppelt , P.	
Fleš , D.: vidi Matijašić , I.	
Florenti , A.: vidi Deacon , G. B.	
Frierson , M. R.: vidi Klopman , G.	
Galabov , B., Nikolova , B. and Orville-Thomas , W. J.: Infrared Band Intensities, Electronic Charge Distribution in Molecules and Polar Properties of Valence Bonds (AR)	1145

XVIII

Galešić, N., Matković, B., Topić, M., Coffou, E. and Šljukić, M. : The Crystal Structure of Disodium Thorium Bisphosphate, $\text{Na}_2\text{Th}(\text{PO}_4)_2$ (OP)	597
Garcia-Leigh, A. and Murrell, J. N. : On the Stability of BH_3 and BF_3 Adducts with BF_3 , CO and N_2 (OP)	879
Gašpert, B. : vidi Djokić, S.	
Geiser, U. : vidi Willett, R. D.	
Gimarc, B. M. : Nonbonded Bond Orders, Molecular Conformations and Relative Stabilities of Sulfur-Nitrogen Rings and Chains (OP)	955
Golič, Lj., Leban, I. and Šegedin, P. : Behaviour of Dimolybdenum Tetraacetate in Aqueous Solutions of Hydrogen Halides. Synthesis and Crystal Structures of $(\text{pyH}_2)[\text{Mo}_2(\text{O}_2\text{CCH}_3)_4\text{Br}_2]$ and Two Modifications of $(\text{pyH}_2)[\text{Mo}_2(\text{O}_2\text{CCH}_3)_4\text{I}_2]$ ($\text{py} = \text{pyridine}$) (OP)	565
Graovac, A. and Polansky, O. E. : Topological Effect on Molecular Orbitals. Part 8. A Study of Two Further Classes of Topological Related Isomers (OP)	1595
Grčev, T. : vidi Cvetkovska, M.	
Grđinić, V. and Jakševac-Mikša, M. : Microdetection of Some Biologically Active Thiol Compounds with Sodium Pentacyanoammineferrate(II) on Ion-Exchange Resin Grains (OP)	411
Grobenski, Z. : vidi Balić Žunić, T.	
Grodzicki, M. : The Applicability of Point-Charge Approximations to the Calculations of Molecular Expectation Values (OP)	1125
Grzonka, M., Knop, J. V., Klasinc, L. and Trinajstić, N. : Theoretical Studies on Small Ring Heteropropellanes. Oxapropellanes (NP)	1629
Gupta, V. K. : vidi Chandravanshi, B. S.	
Habuš, I. : vidi Rapić, V.	
Hada, M. : vidi Nakatsuji, H.	
Haddon, R. C. and Roth, H. D. : Homoconjugation in Radical Cations (OP)	1165
Hadži, D., Hodoček, M., Kocjan, D., Šolmajer, T. and Avbelj, F. : The Molecular Electrostatic Potentials as a Determinant of Receptor-Drug Recognition (OP)	1065
Heilbronner, E. : vidi Honegger, E.	
Herak, J. J. : vidi Kojić-Prodić, B.	
Herak, R. M. : vidi Prelesnik, B. V.	
Herceg, M., Matković, B., Sevdić, D., Matković-Čalogović, D. and Nagl, A. : A Folded Conformation of 1,4,8,11-Tetrathiacyclotetradecane in its Mercury Compound: 1,4,8,11-Tetrathiacyclotetradecanedipicratomercury(II) Heminitromethane, $[\text{Hg}(\text{C}_{10}\text{H}_{20}\text{S}_4) \cdot (\text{C}_6\text{H}_2\text{N}_3\text{O}_7)_2] \cdot 1/2\text{CH}_3\text{NO}_2$ (OP)	609
Hergold-Brundić, A. : vidi Kamenar, B.	
Herman, Z. S. and Pauling, L. : Hybrid Bond Orbitals and Bond Strength for Pentacovalent Bonding (OP)	765
Herndon, W. C. : vidi Szentpály, L. v.	
Hirano, T. and Ōsawa, E. : On the Correspondence between Molecular Orbital Energies and Empirical Force Field Potential Terms (OP)	1633
Hodoček, M., Kocjan, D. and Šolmajer, T. : <i>Ab Initio</i> MO Study of Hydrogen Bonded Complex: Noradrenaline-Formic Acid (OP)	65
Hodoček, M. : vidi Hadži, D.	
Holley, W. W. : vidi Watson, W. H.	
Honegger, E., Yang, Z.-z. and Heilbronner, E. : The Equivalent Bond Orbital Model Revisited: I. Orbitals, Orbital Energies and PE Spectra of Saturated Hydrocarbons (OP)	967
Hoppe, R. : vidi Nowitzki, B.	
Hubač, I. : vidi Kellö, V.	
Hughes, M. : vidi Deacon, G. B.	

Hussain, M. F., Bansal, R. K. and Puri, B. K. : Solid/liquid Separation after Liquid-liquid Extraction: Spectrophotometric Determination of Cobalt By Extraction of its 2-Methoxyethyl Xanthate in Molten Naphthalene (OP)	219
Ip, W.-K. and Li, W.-K. : MNDO Study of the Dimerization of Borane (OP)	1451
Jain, R. : Elucidation of the Structure of Some Potential Antidiabetic Pyrazolin-5-ones Using Polarographic Technique (OP)	235
Jakševac-Mikša, M. : vidi Grdinić, V.	
Jamnický, B. : vidi Mulac-Jeričević, B.	
Jean, Y. : vidi Volatron, F.	
Jug, K. : Bond Order as a Tool for Molecular Structure and Reactivity (AR)	941
Julg, A. : The Problem of Enantiomers: Support for a New Interpretation of Quantum Mechanics (OP)	1497
Julg, A. and Deprick, B. : Theoretical Study of Adsorption of Carbonyl Compounds on Ionic Crystals: I. Formaldehyde, Glyoxal, o- and p-Benzoinone on the (100) Face of Sodium Chloride (OP)	85
Kálmán, A., Argay, G., Ribár, B., Vladimirov, S. and Živanov-Stakić, D. : Crystal and Molecular Structure of 3β -Hydroxy- $14,15\beta$ -epoxy- 5β -card-20,22-enolide (Digirezigenin) (OP)	519
Kamenar, B., Penavić, M. and Hergold-Brundić, A. : The Crystal Structure of Phenylmercury(II) Trifluoroacetate and the Refinement of the Crystal Structure of Phenylmercury(II) Acetate (OP)	145
Kamenar, B., Penavić, M. and Marković, B. : The Crystal Structure of Piridinium μ -salicylato-tetrachloro- μ -oxo- μ -ethoxo-dioxodimolibdate(V) (OP)	637
Kang, S.-K., Albright, T. A. and Silvestre, J. : The Bonding of P_4 to d^8 -ML ₃ Complexes (OP)	1355
Kapur, V. : vidi Dua, S. K.	
Kapuy, E., Csépes, Z. and Kozmutza, C. : Many-Body Perturbation Theory Based on Localized Orbitals (AR)	855
Keglević, D. : vidi Mulac-Jeričević, B.	
Kellö, V., Hubač, I., Boldyrev, A. I. and Špirko, V. : <i>Ab Initio</i> MBPT(4) Calculations of the Inversion Potential Function of NH ₃ (OP)	1661
Kibler, M. : Symmetry Adaptation and Wigner-Racah Algebras in Quantum Chemistry (AR)	1075
Kibler, M. and Négadi, T. : On the Use of Nonbijective Canonical Transformations in Chemical Physics (OP)	1509
Kidrič, J. : vidi Kobe, J.	
Kirtman, B. and Palke, W. E. : Factors Governing Nuclear Geometry and Bond-Orbital Directions in Second Row AM ₂ Molecules (OP)	1247
Klasinc, L. : vidi Grzonka, M.	
Klessinger, M. : Fragment Molecular Orbitals for Molecules and Interacting Systems (AR)	887
Klopman, G. and Frierson, M. R. : The Alpha-Effect. A Theoretical Study Incorporating Solvent Effects (OP)	1411
Knop, J. V. : vidi Grzonka, M.	
Kobe, J., Crnjak Orel, T. and Kidrič, J. : Complex Formation Between the Antiviral Nucleoside Ribavarin (1- β -D-Ribofuranosyl-1,2,4-Triazole-3-Carboxamide) and Bivalent Metal Ions: ¹ H and ¹³ C NMR Studies, and Comparison with Inosine (OP)	165
Kobe, J., Rusjakovski, B. and Brdar, B. : The Synthesis and Antiviral Activities of 2-Substituted Azino-3- β -D-ribofuranosyl and α and β -D-arabinofuranosyl-5-carbamoylmethylenethiazolidine-4-ones (OP)	295
Kocjan, D. : vidi Hodošček, H. Hadži, D.	
Kojić-Prodić, B., Ružić-Toroš, Ž., Snatzke, G. and Herak J. J. : An Absolute Configuration of (1R, 4R, 5R)-4-Methoxy-8-acetyl-7,7-dimethyl-6-thia-3,8-diazabicyclo[2.2.1]octan-2-one, C ₁₀ H ₁₆ N ₂ O ₃ S (OP)	661

Korpar-Čolig, B., Popović, Z. and Sikirica, M. : Mercuration of Some Aliphatic Aldehydes. The Crystal Structure of 2,2-Bis(chloromercuri)butyraldehyde (OP)	689
Koukoulas, A. and Whitehead, M. A. : Penetration in the CNDO Theory (OP)	1225
Kovačević, K., Maksić, Z. B. and Moguš-Milanković, A. : Geometry of Molecules. Part 7. Interatomic Distances, Bond Angles and Strain Energies in Some Rotenes and Related Spirocompounds by the IMO Method (OP)	187
Kezumtza, C. : vidi Kapuy, E.	
Kraka, E. : vidi Cremer, D.	
Krivka, P. : vidi El-Basil, S.	
Krygowsky, T. M., Wieckowski, T. and Sokolowska, A. : Infrared and Raman Studies of Carbonyl Group Frequencies of <i>p</i> -Substituted Benzoic Acids in the Crystalline State (OP)	229
Kujundžić, N. : vidi Biruš, M.	
Kuz'mina, L. G. and Struchkov, Y. T. : Structural Chemistry of Organomercury Compounds. Role of Secondary Interactions (AR)	701
Kvasnička, V. : Second-Quantization Formalism for Geminals (OP)	1643
Kveder, S. : vidi Mulac-Jeričević, B.	
Ladika, M. and Sunko, D. E. : Allylic Cations in Solvolysis. A Case of Non-Participation (PC)	179
Ladika, M., Sunko, D. E. and Borčić, S. : Solvolysis Rate of 3-Methyl-2-(3-pentynyl)-2-cyclohexenyl <i>p</i> -Nitrobenzoate. A Model System for π -Participation of the CC Triple Bond (OP)	331
Lah, T. : vidi Babnik, J.	
Larkins, F. P. : vidi Deacon, G. B.	
Larson, J. R. : vidi Epiotis, N. D.	
Lasić, D. D., Marcondes, M. E., Reeves, L. W. and Szarka, M. : Micelle Forms in Lyotropic Nematics and Cholesterics (OP)	129
Lazar, D. : vidi Radivojević, P.	
Leban, I. : vidi Golič, Lj.	
Lee, S. : vidi Burdett, J. K.	
Li, W.-K. : vidi Ip, W.-K.	
Lingafelter, E. C. : vidi Elia, A. E.	
Lovrić, M., Magjer, T. and Branica, M. : Electrochemical Kinetic Measurements and Metal Speciation with the Vibrating Dropping Mercury Electrode (OP)	153
Luken, W. L. : Properties of the Fermi Hole in Molecules (OP)	1283
Lukić, I. : vidi Djokić, S.	
Maasböl, A. G. : vidi Djokić, S.	
Mackay, A. L. : Descriptors for Complex Inorganic Structures (OP)	725
Magjer, T. : vidi Lovrić, M.	
Maksić, Z. B., Eckert-Maksić, M. and Rupnik, K. : Model Description of Some Molecular Properties by the Modified-Atom-in-a-Molecule (MAM) Approach (AR)	1295
Maksić, Z. B. : vidi Kovačević, K.	
Malinar, M. J., Radivojša, P. N., Marković, K., Belić, D. and Čelap, M. B. : Synthesis and Configuration of New Isomers of the Bis(aminocarboxylato)carbonatocobaltate(III) Ion (OP)	443
Mandić, Z. : vidi Djokić, S.	
Manojlović-Muir, Lj. and Muir, K. W. : A Novel Pt(II)—Pt(IV) Mixed Valence Complex: The Crystal and Molecular Structure of $[LP(\mu-I)(\mu-\text{Me}_2\text{PCH}_2\text{PMc}_2)_2\text{PtMe}_3][I_3]$, $L=0.45I+0.55\text{Me}$ (OP)	587
Marcondes Helene, M. E. : vidi Lasić, D. D.	
Marković, B. : vidi Kamenar, B.	

Marković, K.: vidi Malinar, M. J.	
Matijašić, I., Andreotti, G. D., Sgarabotto, P., Bezjak, A. and Fleš, D.: Crystal and Molecular Structure of (S)- α -(<i>p</i> -Bromobenzenesulphonamido)- β -propiothiolactone (OP)	621
Matković, B.: vidi Galešić, N.; Herceg, M.	
Matulić-Adamić, J.: vidi Škarić, V.	
McWeeny, R.: Weak Interactions Between Molecules (OP)	865
Meider, H.: vidi Bronzan-Planinić, P.	
Mesarić, Š.: vidi Brničević, N.	
Milat, O.: vidi Težak, Đ.	
Milinski, N.: vidi Radivojević, P.	
Moffat, J. B.: Partitioning and Additivity of the Chemical Bond (OP)	1475
Moguš-Milanović, A.: vidi Topić, M., Kovačević, K.	
Muir, K. W.: vidi Manojlović-Muir, Lj.	
Mulac-Jeričević, B., Vranešić, B., Kveder, S., Jamnický, B. and Keglević, D.: Crystalline Suspension of Bovine Zinc Des-AlaB30-Insulin with Prolonged Hypoglycaemic Activity (OP)	289
Murrell, J. N.: vidi Carter, C.; Garcia-Leigh, A.	
Nagl, A.: vidi Herceg, M.	
Nakatsuji, H. and Hada, M.: Interaction of the Hydrogen Molecule with the Palladium Atom. A Force Theoretic Study (OP)	1371
Náray-Szabó, G.: Chemical Fragmentation for Molecular Orbital Calculations on Proteins (OP)	901
Nardelli, M.: vidi Battaglia, L. P.	
Négadi, T.: vidi Kibler, M.	
Nikolova, B.: vidi Galabov, B.	
Nowacki, W.: vidi Engel, P.	
Nowitzki, B. and Hoppe, R.: Eine Bemerkung über $K_2[NiO_2]$ (OP)	537
Orbell, J. D.: vidi Bresciani-Pahor N.	
Ortoleva, E. and Simonetta, M.: A Theoretical Study of the Influence of Surface Structure on Chemisorption of Nitrogen on Iron Single-Crystal Faces (OP)	1387
Orville-Thomas, W. J.: vidi Galabov, B.	
Ōsawa, E.: vidi Hirano, T.	
Palke, W. E.: On Determining Orbital Hybridization (OP)	779
Palke, W. E.: vidi Kirtman, B.	
Pauling, L.: vidi Herman, Z. S.	
Pavela-Vrančić, M.: vidi Škarić, V.	
Penavić, M.: vidi Kamenar, B.	
Persico, M. and Tomasi, J.: An Evaluation of Solvent Effects on Isomerization Mechanisms in Diimide and Methylenimine (OP)	1395
Petrongolo, C.: Non Adiabatic Effects and Radiationless Transition (OP) . .	1485
Petrov, G.: vidi Cvetkovska, M.	
Polansky, O. E.: vidi Graovac, A.	
Politzer, P. and Zilles, B. A.: Some Observations Concerning Electronic Densities, Electrostatic Potential and Chemical Potential (OP)	1055
Popović, S.: Application of Bell-Shaped Functions in X-ray Diffraction Broadening Analysis (OP)	749
Popović, Z.: vidi Korpar-Čolig, B.	
Prelesnik, B. V. and Herak, R. M.: The Crystal Structure of <i>trans</i> (NO ₂ , N=C—CH ₃)-(N-ethylidene-ethylenediamine)-glycylglycinatonitrocobalt (III) Monohydrate, [Co(glygly)-NO ₂ (CH ₃ CH=en)]·H ₂ O (OP)	577

Pribanić, M.: vidi Biruš M.	
Proštenik, M. V., Dumić, M. and Butula, I.: Chemistry of 1,3-Dioxepins. II. Dehydrohalogenation of 5,6-Dihalogen-1,3-Dioxepanes with Strong Bases (OP)	281
Proštenik, M. V.: vidi Dumić, M.	
Puri, B. K.: vidi Hussain, M. F.	
Pušelj, M., Ban, Z. and Szitula, A.: The Crystal Structure and Magnetic Properties of the Cu ₂ MnAl _{1-x} Hg _x System (OP)	669
Radivojević, P., Milinski, N., Ribár, B. and Lazar, D.: The Crystal Structure of the Complex [Y(H ₂ O) ₅ (NO ₃) ₂] [Y(H ₂ O) ₂ (NO ₃) ₄] (OP)	451
Radivojša, N.: vidi Malinar, M. J.	
Randaccio, L.: vidi Bresciani-Pahor, N.	
Raos, N. and Simeon, Vl.: Conformational Analysis of Bis(N,N-dimethylisoleucinato)-Copper(II): Estimation of the Diastereoselectivity Effect by Means of two Approximate Methods (OP)	1217
Rapić, V. and Habuš, I.: Ferrocene Compounds. XII. Reactions of Ferrocenecarbaldehyde with Benzanilides and n-Butyllithium (OP)	265
Reevs, L. W.: vidi Lasič, D. D.	
Ribár, B.: vidi Kálmán, A.; Radivojević, P.	
Roth, H. D.: vidi Haddon, R. C.	
Rupnik, K.: vidi Maksić, Z. B.	
Rusjakovski, B.: vidi Kobe, J.	
Ružić-Toroš, Ž.: vidi Kojić-Prodić, B.	
Sahni, S. K.: vidi Dua, S. K.	
Schäfer, H.: vidi Brničević, N.	
Schomaker, V.: vidi Elia, A. E.	
Sevdić, D.: vidi Herceg, M.	
Sgarabotto, P.: vidi Matijašić, I.	
Sha, W. C.: vidi Burdett, J. K.	
Sherrod, R. E.: vidi Bloor, J. E.	
Siew, P. Y.: vidi Alyea, E. C.	
Sikirica, M.: vidi Korpar-Čolig, B.	
Silvestre, J.: vidi Kang, S.-K.	
Simeon, Vl.: vidi Raos, N.	
Simonetta, M.: vidi Ortoleva, E.	
Skancke, P. N.: A Molecular-Orbital Study of the Thermal Walk Rearrangement of Bicyclo[2.1.0]-pent-2-ene (OP)	1445
Snatzke, G.: vidi Kojić-Prodić, B.	
Sokolowska, A.: vidi Krygowsky, T. M.	
Spanget-Larsen, J.: Breakdown of the One-Electron Picture of Ionization for Hydrocarbon π-Systems (OP)	991
Stanley, A. E.: vidi Colombo, L..	
Stradella, O. G.: vidi Villar, H. O.	
Strajnar, F.: vidi Težak, Đ.	
Struchkov, Y. T.: vidi Kuz'mina, L. G.	
Stubičar, M.: vidi Težak, Đ.	
Sundell, R.: vidi Beno, M. A.	
Sunko, D. E.: vidi Ladika, M.	
Surján, P. R.: The Representation of the Chemical Bond in Quantum Chemical Calculations (OP)	833
Szarka, M.: vidi Lasič, D. D.	
Szentpály, L. v. and Herndon, W. C.: A Comparison of Pencil and Paper Procedures. PMO, Free Electron PMO, and Structure-Resonance Theory Calculations of Proton Affinities (OP)	1621

Szitula, A.: vidi Pušelj, M.	
Šarčević, D.: vidi Težak, Đ.	
Šćavničar, S.: vidi Balić Žunić, T.	
Šegedin, P.: vidi Golič, Lj.	
Šimaga, Š.: vidi Šunjić, V.	
Šimunić, B.: vidi Dokić, S.	
Škarić, V. and Škarić, D.: Novel Syntheses of Thiazolo[3,2-a]pyrimidin-7-ones (PC)	183
Škarić, V. Pavela-Vrančić, M. and Matulić-Adamić, J. : Stereoselective Transformations in the Tymidine Series (OP)	415
Škarić, Đ.: vidi Škarić, V.	
Šljukić, M.: vidi Galešić, N.	
Šolmajer, T.: vidi Hadži, D.	
Špirko, V.: vidi Kellö, V.	
Sunjić, V., Šimaga, Š. and Vitale, Lj.: The Synthesis and Angiotensin Converting Enzyme Inhibitory Activities of <i>N</i> -(3-Substituted)aminocarbonyl]-propanol-L-prolines (OP)	251
Tabor, Z.: vidi Biruš, M.	
Težak, Đ., Strajnar, F., Šarčević, D., Milat, O. and Stubičar, M.: Solid/Liquid Equilibria in Aqueous Systems of Dodecyl Benzene Sulphonate and Alkaline Earth Ions (OP)	93
Thulstrup, E. W.: Interpretation of Optical Spectra of Partially Aligned Samples (AR)	1667
Tomasi, J.: vidi Persico, M.	
Tomescu, I.: vidi Balaban, A. T.	
Tomić, M.: vidi Djokić, S.	
Tonachini, G.: vidi Bernardi, F.	
Topić, M. and Moguš-Milanković, A.: A Multiple Thermal Analysis of Ammonium Heptamolybdate Tetrahydrate (OP)	75
Topić, M.: vidi Galešić, N.	
Trinajstić, N.: vidi El-Basil, S.; Grzonka, M.	
Trindle, C.: The Hierarchy of Models in Chemistry (OP)	1231
Turk, V.: vidi Babnik, J.	
Tušek-Božić, Lj. and Božić, B.: Conductance Study of Ion-Pairing of Alkali Picrate and Tetraphenylborate Complexes with Some Macrocyclic Polyethers in Methanol (OP)	119
Vasić-Rački, Đ.: Immobilization of Yeast Alcohol Dehydrogenase on Weakly Basic Anion Exchange Resin Beads (OP)	305
Villar, H. O., Stradella, O. G., Cachau, R. E. and Castro, E. A.: Some Comments on the Nucleation Phenomena (OP)	1417
Vitale, Lj.: vidi Šunjić, V.	
Vladimirov, S.: vidi Kálmán, A.	
Vogler, H.: Donor-Acceptor Cyclophanes with Biradical-Ionic Ground States (OP)	325
Vogler, H.: A Theoretical Study of the ¹ H-Chemical Shifts of [4n]- and [4n+2]Annulenes and their Di- and Tetraanions (OP)	1177
Volatron, F., Jean, Y. and Anh, Ngyén T.: The Role of Lone Pairs in Heteroatomic Chemistry. Graphical Analysis and <i>Ab Initio</i> Calculations of Oxirane and Aziridine Ring Opening (OP)	1461
Vranešić, B.: vidi Mulac-Jeričević, B.	
Vučković, D. Lj. and Vujišić, Lj.: Structure and Properties of Small Ring Propellanes by the IMO Method (OP)	801

XXIV

- Vujisić, Lj.: vidi Vučković, D. Lj.
- Watson, W. H. and Holley, W. W.: The Structure of Four Complexes of 2,2,6,6-Tetramethyl-3,5-heptanedione Containing One, Four, Four and Nine Cu(II) Ions (**OP**) 467
- Weinberg, N. N.: vidi Basilevsky, M. V.
- Weiss, R.: vidi Doppelt, P.
- Whithead, M. A.: vidi Koukoulas, A.
- Wieckowski, T.: vidi Krygowski, T. M.
- Willett, R. D. and Geiser, U.: Structural Characteristics of ACuCl₃ Salts (**OP**) 737
- Williams, J. M.: vidi Beno, M. A.
- Zhulin, V. M.: vidi Basilevsky, M. V.
- Zilles, B. A.: vidi Politzer, P.
- Živanov-Stakić, D.: vidi Kálmán, A.
- Živković, T. P.: Splitting of the Configuration Interaction Space X_n into Two Complementary Subspaces (**OP**) 367
- Živković, T. P.: The Splitting Theorem and Properties of Alternant Systems (**OP**) 1553
- Živković, T. P.: Antialternant Perturbations of Alternant Systems (**OP**) 1575
- Yang, Z.-z.: vidi Honegger, E.