

Contents of Vol. 82

ORIGINAL SCIENTIFIC PAPERS

M. Hurtado, O. Mó, M. Yáñez, and J.-C. Guillemin: Acidity Enhancement of the Cyclopentadiene Ring by PH₂ and AsH₂ Substitution..... 1–6

C. Matthias and D. Kuck: Gaseous [C_nH_{2n+1}⁺ ... 1,3-Diphenylpropane] Ion/Neutral Complexes Containing Alkyl Cations of Different Acidities and Hydride Ion Affinities..... 7–19

M. Dimitrova and B. Galabov: Predicting the Acidities of Substituted Phenols Using Electrostatic Potential at Nuclei 21–25

R. Vianello: Acidifying Effect of an *N*-Oxide Group – A Useful Motif in Enhancing Acidity towards Superacidic Values..... 27–39

Zh. Tian, A. Fattahi, L. Lis, and S. R. Kass: Neutral Intramolecular Hydrogen-bonded Bases 41–45

G. Bouchoux and R. X. Chia: Gas-phase Basicity of Glycine 47–61

Z. Glasovac, M. Vazdar, and D. Margetić: Proton Affinities of Didehydroporphyrin and Subporphyrin in Ground and Excited States Obtained by Quantum Chemical Calculations..... 63–70

P. Burk, K. Taul, and J. Tammiku-Taul: Proton and Lithium Cation Binding to Some β-Dicarbonyl Compounds. A Theoretical Study 71–77

J. Mišek, M. Tichý, I. G. Stará, I. Starý, J. Roithová, and D. Schröder: Assembling Screws: Large Preference for the Homochiral Combination in the Proton-Bound Dimers of 1-Aza[6]helicene in the Gas Phase..... 79–86

E. D. Raczyńska, J.-F. Gal, P.-C. Maria, and M. Szelağ: Proton Transfer Chemistry in the Gas Phase. Is a Spontaneous 'Neutralization' Reaction a Myth or a Reality?..... 87–103

A. J. A. Aquino, F. Plasser, M. Barbatti, and H. Lischka: Ultrafast Excited-state Proton Transfer Processes: Energy Surfaces and On-the-fly Dynamics Simulations..... 105–114

I. Hyla-Kryspin, C. Mück-Lichtenfeld, and S. Grimme: DFT Studies on Molecular and Electronic Structures of Cationic Carbene Complexes [L₂(η⁵-C₅H₅)Fe=CR₅]⁺ (L = CO, PH₃, dhpe, PPh₃; R = H, F, CH₃)..... 115–127

P. López-Tarifa, F. Martín, M. Yáñez, and M. Alcamí: Theoretical Study of Doubly Charged [X(H₂O)] and [X(NH₃)] (X = Si, Ge, Sn, Pb) Molecular Ions 129–137

M. A. Dobrowolski, T. M. Krygowski, and M. K. Cyrański: Substituent Constants (σ_p⁻) of the Rotated Nitro Group. The Interplay Between the Substituent Effect of a Rotated –NO₂ Group and H-Bonds Affecting π-Electron Delocalization in 4-Nitrophenol and 4-Nitrophenolate Complexes: a B3LYP/6-311+G** Study 139–147

J. E. Del Bene, O. Mó, and M. Yáñez: Substituent Effects on B–N Bonding and Coupling Constants in Five-membered Rings N₃B₂H₄X and N₂B₃H₄X, for X = H, F, and Li..... 149–155

N. Sablon, F. de Proft, and P. Geerlings: Reformulating the Woodward-Hoffmann Rules in a Conceptual Density Functional Theory Context: the Case of Sigmatropic Reactions 157–164

C. A. Deakyne, L. H. Warfel IV, H. M. Thomas, D. Nauduri, T. E. A. Ajibowo, N. J. Carbonaro, A. G. Simpson, and J. F. Liebman: The Energetics of Halogenated Ethylenes (Ethyne)s and 1,3-Butadienes (Butadiynes): A Computational and Conceptual Study of Substituent Effects and “Dimerization” 165–172

F. Blanco, I. Alkorta, and J. Elguero: Barriers about Double Carbon-Nitrogen Bond in Imine Derivatives

- (AlDIMINES, Oximes, Hydrazones, Azines) 173–183
- S. J. Grabowski:** Covalent Character of Hydrogen Bonds Enhanced by π -Electron Delocalization . 185–192
- S. Duley, P. Goyal, S. Giri, and P. Kumar Chattaraj:** Bonding, Reactivity and Aromaticity in Some Beryllocene Derivatives 193–205
- B. Xu, Q.-S. Li, Y. Xie, B. King, and H. F. Schaefer III:** Heptacarbonyldiosmium and Hexacarbonyldiosmium: Two Highly Unsaturated Binuclear Osmium Carbonyls 207–218
- G. F. Caramori and G. Frenking:** The Effects of N-Heterocyclic Ligands on the Nature of the Ru–(NO) Bond in Ruthenium Tetraammine Nitrosyl Complexes .. 219–232
- E. Kraka, M.I Filatov, and D. Cremer:** Comparison of Gold Bonding with Mercury Bonding 233–243
- R. D. Harcourt:** On the Magnetic Exchange Parameter for an O–Cu–Cu–O Component of Cu^{II} Carboxylate Dimers 245–251
- L. Éhn, I. Černušák, and P. Neogrady:** Dipole Polarizabilities of Fluorinated Hydrocarbons 253–259
- J. F. Liebman and Z. S. Herman:** On the Angular Independence of Sets of Atomic Orbitals 261–265
- J. S. Murray and P. Politzer:** Molecular Surfaces, van der Waals Radii and Electrostatic Potentials in Relation to Noncovalent Interactions 267–275
- V. Harmat and G. Náráy-Szabó:** Theoretical Aspects of Molecular Recognition 277–282
- J. M. del Campo and A. M. Köster:** The Importance of Step Control in Optimization Methods 283–290
- M. K. Kesharwani and B.t Ganguly:** Solvent Effects on the Stereoselectivity of Reaction of Methyl Acrylate, Methyl Methacrylate and Methyl *trans*-Crotonate with Cyclopentadiene: A Computational Study 291–298
- B. Furlan, S. Golič Grdadolnik, S. Hočevar, D. Kocjan, J. Levec, H. Maskill, H. Navrátilová, J. Pospíšil, M. Potáček, U. Urleb, and J. Žmitek:** Amlodipine Benzenesulfonate: A Mechanistic Investigation of Its Industrial Preparation via Detritylation of *N*-tritylamlopidine and Related NMR Studies 299–309
- J. H. A. Al-Fahemi, D. L. Cooper, and N. L. Allan:** Predictions of Toxicity to *Chlorella vulgaris* and the Use of Momentum-space Descriptors 311–316
- M. Kržan and J. Mavri:** Carcinogenicity of Styrene Oxide: Calculation of Chemical Reactivity 317–322
- N. Kallay, T. Preočanin, A. Selmani, F. Šupljika and I. Leniček:** High Resistance Compensation Method for Surface Potential Measurement 323–327
- G. Pehnc, L. Klasinc, G. Šorgo, and V. Vadić:** Analysis of Summer 2006 Ozone Pollution in Zagreb 329–335
- D. Milić, Ž. Soldin, G. Giester, Z. Popović, and D. Matković-Čalogović:** Crystal Structure of the First Polymeric Tetramercurated Methane Derivative of Hofmann's Base 337–344
- K. Molčanov, B. Kojić-Prodić, and A. Meden** Unique Electronic and Structural Properties of 1,4-Benzoquinones: Crystallochemistry of Alkali Chloranilate Hydrates 387–396
- M. Ristić, S. Popović, and S. Musić:** Investigation of Crystalline Phases in the $\alpha\text{-Fe}_2\text{O}_3/\alpha\text{-Al}_2\text{O}_3$ System 397–404
- Ž. Skoko, S. Popović, and G. Štefanić:** Microstructure of Al-Zn and Zn-Al Alloys 405–420
- B. Prugovečki, E. J. Dodson, G. G. Dodson, and D. Matković-Čalogović:** Structure of the T_6 Human Nickel Insulin Derivative at 1.35 Å Resolution 433–438
- G. Mikleušević, B. Salopek-Sondi, and M. Luić:** Arab-1, a GDSL Lipase from the Model Plant, *Arabidopsis thaliana* (L.) Heynh. 439–447
- A. Pifferi, G. Campi, C. Giacobozzo, and E. Gobbi:** A New Portable XRD/XRF Instrument for Non-destructive Analysis 449–454
- B. Kozlevčar, I. Kovšca, Z. Jagličić, A. Pevec, N. Kitanovski, P. Strauch, and P. Šegedin:** Strong Antiferromagnetism in Isolated Anionic Dicopper(II) Methanoato *Paddle-wheel* Complex 463–467
- P. Novak, K. Pičuljan, T. Hrenar, and V. Smrečki:** Structure and Hydrogen Bonding Interactions in Methoxysalicylaldehyde Thiosemicarbazone Derivatives in Solution by NMR and DFT Methods 477–483
- E. Zupanič, R. Žitko, H. J. P. van Midden, I. Mušević, and A. Prodan:** Low-temperature Scanning Tunneling Microscopy and Spectroscopy of Noble-metal Surfaces 485–491
- N. Kallay, T. Preočanin, and D. Kovačević:** Effect of Charge Distribution on the Stability of Nano-dispersions 531–535
- B. Zhou and N. Trinajstić:** On Reciprocal and Reverse Balaban Indices 537–541
- G. Pehnc, L. Klasinc, V.r Vadić, and G. Šorgo** Estimation of Ozone and Peroxide Levels in the Air of Croatia 543–551
- V. Gvozdić, V. Tomišić, V. Butorac, and V. Simeon:**

- Association of Nitrate Ion with Metal Cations in Aqueous Solution: a UV-Vis Spectrometric and Factor-Analytical Study 553–559
- A. Tomić and T. P. Živković:** On the Vibrational Interlacing Rule in Deuterated Thiophene: I. Out-of-plane Vibrations 561–566
- N. Kitanovski, A. Golobič, and B. Čeh:** Two Compounds with *trans*-[Mo(NCS)₄(γ -pic)₂][−] Anion. 567–571
- E. Biçer and P. Çetinkaya:** Electrochemical Behaviour of the Antibiotic Drug Novobiocin Sodium on a Mercury Electrode 573–582
- E. Biçer and C. Arat:** A Voltammetric Study on the Aqueous Electrochemistry of Acid Red 1 (Azophloxine) 583–593
- R. Hefferlin:** Two Descriptors for Series of Congeneric Molecules 595–598
- M. A. Kamyabi, and F. Aghajanloo:** Electrocatalytic Response of Dopamine at a Carbon Paste Electrode Modified with Ferrocene 599–606
- D. Kushev, V. Enchev, E. Naydenova, R. Detcheva, N. Spassovska, and K. Grancharov:** Synthesis, Structure and Cytotoxicity of Platinum(IV) Complexes of 3-Aminocyclohexanespiro-5-hydantoin and 3-Aminocycloheptanespiro-5-hydantoin 607–611
- K. Mitka, P. Kowalski, D. Pawelec, Z. Majka:** Synthesis of Novel Indane-1,3-dione Derivatives and Their Biological Evaluation as Anticoagulant Agents 613–618
- L.-T. Pan, X.-H. Liu, and H.-W. Gao:** Complexation between Antimony and *o*-Chlorophenylfluorone and its Application to Determination of Antimony in Wastewater 619–622
- S. Chibowski, E. Grządka, and J. Patkowski:** Influence of a Type of Electrolyte and its Ionic Strength on the Adsorption and the Structure of Adsorbed Polymer Layer in the System: Polyacrylic Acid/SiO₂ 623–631
- A. Miličević and N. Raos:** Estimation of Stability Constants with Connectivity Index: Development of Bivariate and Multivariate Linear Models for Copper(II) Chelates with Oligopeptides 633–639
- S. Li, X. Li, and Z. Zhuc:** Hosoya Indices of Bicyclic Graphs 641–647
- J. Cz. Dobrowolski:** The Homology Relation between Molecules a Revival of an Old Way for Classification of Molecules 649–661
- L. P. Schulz:** Mathematical Patterns in Chemistry – on Turn Points in the Molecular Self-Assemblage Symmetry Formation 663–677
- B. Horvat:** On the Calculation of the Terminal Polynomial of a Star-like Graph 679–684
- R. Injac, N. Kocevar, B. Strukelj:** Optimized Method for Determination of Amoxicillin, Ampicillin, Sulfamethoxazole, and Sulfacetamide in Animal Feed by Micellar Electrokinetic Capillary Chromatography and Comparison with High-Performance Liquid Chromatography 685–694
- J. Li, Y. Zhang, X. Wang, and Y.-S. Ho:** Bibliometric Analysis of Atmospheric Simulation Trends in Meteorology and Atmospheric Science Journals 695–705
- V. Butković:** Nitroxide Mediated Degradation of Anthocyanidins 707–713
- A. Fajdetić, G. Kobrehel, G. Lazarevski, Z. Marušić-Ištuk, and S. Mutak:** Synthesis and Structural Properties of Novel Tricyclic 15-membered Azalides .. 715–723
- M. A. Karimi, M. Mazloum-Ardakani, M. H. Mashhadizadeh, and F. Banifateme:** Simultaneous Kinetic Spectrophotometric Determination of Hydrazine and Isoniazid Using H-Point Standard Addition Method and Partial Least Squares Regression in Micellar Media 729–738
- J. Sabotič, T. Popovič, and J. Brzin:** Aspartic Proteases from Basidiomycete *Clitocybe nebularis* 739–745
- M. V. N. Padma Rao, L. S. Rao, M. S. Reddy, V. R. Kumar, and N. Veeraiyah:** Magnetic and spectroscopic studies on molybdenum ions in CaF₂-PbO-P₂O₅ glass system 747–752
- A. Niazi, A. Yazdanipour, J. Ghasemi, M. Kubista, A. Sheyda, and M. Alikhah:** Spectrophotometric Determination of the Dissociation Constants of Fluorescein in Micellar Media 753–757
- C. G. Laudani, M. Primožič, Ž. Knez, and M. Habulin:** Phase Equilibrium Measurements and Data Correlation for the Ternary System Oleic Acid + 1-Octanol + Carbon Dioxide 761–769
- B. Horvat, T. Pisanski, and A. Žitnik:** The Dilation Coefficient of Complete Graphs 771–779
- G. Brinkmann, O. Delgado-Friedrichs, E. C. Kirby, and N. Van Cleemput:** A Catalogue of Periodic Fully-Resonant Azulene-Transitive Azulenoid Tilings Analogous to Clar Structures 781–789
- M. Randić:** Positronium – Hydrogen Like and Unlike... 791–800
- M. Buzuk, S. Brinić, E. Generalić, and M. Bralić:**

Copper(II) ion selective PVC membrane electrode based on S,S'-bis(2-aminophenyl)ethanebis(thioate).... 801-806

A. Budimir, E. Bešić, and M. Biruš: Kinetics and Mechanism of Oxidation of Hydroxyurea with Hexacyanoferrate(III) Ions in Aqueous Solution 807-818

K. Gunasekar and K. Anbarasu: Linear Free Energy Relationships in the Chromium(VI) Oxidation Of Phenols 819-823

Lj. Tomašek, A. Jukić and Z. Janović: Free radical grafting of methyl methacrylate onto ethylene-propylene amorphous copolymer 825-832

D. Milić, M. Alešković, D. Matković-Čalogović, and K. Mlinarić-Majerski: (1-Adamantyl)methyl esters: whole-molecule disorder in the crystal structure of (1-adamantyl)methyl-1-adamantanecarboxylate..... 833-839

NOTE

Ž. Maleš, M. Plazibat, and F. Bucar: Essential Oil of *Portenschlagiella ramosissima* from Croatia, a Rich Source of Myristicin..... 725-728

PRELIMINARY COMMUNICATION

S. Kazazić, S. P. Kazazić, and D. Srzić: Gas-phase Ligation of Cr⁺/ Fe⁺/ Ni⁺ Ions with Iodine 841-843

REVIEW

A. Thumiger and G. Zanotti: Iterative Methods for the Solution of the Phase Problem in Protein Crystallography..... 421-432

B. Kotur, O. Myakush, and I. Zavaliy: Hydrogen Sorption Properties of Some $RM_{2-x}M'_x$ and $RM_{2-x}Al_x$ (R = Y, Gd, Tb, Er, Ho; M = Mn, Fe, Co, Ni) Laves Phase Ternary Compounds 469-476

AUTHOR'S REVIEW

M. Cindrić, Z. Veksli, and B. Kamenar: Polyoxomolybdates and Polyoxomolybdovanadates – from Structure to Functions: Recent Results 345-362

G. Jovanovski, P. Makreski, B.o Kaitner, and B. Boev: Silicate Minerals from Macedonia. Complementary Use of Vibrational Spectroscopy and X-ray Powder Diffraction for Identification and Detection Purposes.....

363-386

R. Dreos, L. Randaccio, P. Siega, and V. Vrdoljak: Intramolecular Cyclization Reactions in Haloalkyl-Cobalt Complexes with Macrocyclic Equatorial Ligands 455-461

S. Bilokapić, N. Ban, and I. Weygand-Đurašević: Seryl-tRNA Synthetases: Enzymes with Multiple Personalities 493-501

V. Šunjić: Separation of Enantiomers by Chromatography as a Vehicle for Chiral Catalysis. Abridged Review. 503-530

PREFACES

D. Margetić and R. Vianello: Editorial CI-CXVII

R. Vianello and D. Margetić: Scientific Journey of Zvonimir Maksić CXIX-CXXXI

M. Cindrić and B. Kamenar: Editorial CCXV

B. Kamenar: DRAGO GRDENIĆ – *Curriculum Vitae* . CCXVII-CCIX

M. Cindrić: DRAGO GRDENIĆ – *List of Publications* CCXXI-CCXXIV

APPENDICES

Book ReviewCXXXIII-CXXXIV, CCCI-CCCII

Instructions to Authors CXXXV-CXXXIX

Contents of Croatica Chemica Acta Vol.82 CCCCIX-CCCCXII