

CROATICA CHEMICA ACTA

Croat. Chem. Acta Vol. 69 No. 3

XI–XIV, 741–1274, A1–A2, C9–C10 (1996)

Zagreb, November, 1996

CONTENTS

Proceedings of the Tenth Dubrovnik International Course and Conference
MATH/CHEM/COMP, Dubrovnik 1995

FOREWORD	... Ante Graovac	XI–XII
Dubrovnik 1995 (poem)	... Mircea V. Diudea	XII

Enumeration and Computation

The Column-Convex Polyominoes Perimeter Generating Function for Everybody	... Svjetlan Feretić	741–756
Unbranched Catacondensed Polygonal Systems Containing Hexagons and Tetragons	... Sven J. Cyvin, Björg N. Cyvin, and Jon Brunvoll	757–774
A New Algorithm for Global Minimization Based on the Combination of Adaptive Random Search and Simplex Algorithm of Nelder and Mead	... Miljenko Huzak and Željko Bajzer	775–791
Polymer Chains in Random Layered Flows: A Scaling Approach	... Jens-Uwe Sommer and Alexander Blumen	793–803

Group Theory and Topology in Chemistry

Crystallographic and Quasicrystallographic Lattices from the Finite Groups of Quaternions	... R. Bruce King	805–812
Topology and Group Theory-Tools for Determinating the Stereochemistry of Molecules	... Stefan Reichelt, Antje Reichelt, Nicole Müller, and Ivar Ugi	813–825
Geometry <i>versus</i> Topology: Testing Self-Consistency of the NiceGraph Program	... Tomaž Pisanski, Marko Razinger, and Ante Graovac	827–836
Computing the Szeged Index	... Janez Žerovnik	837–843
On the Szeged Index of Unbranched Catacondensed Benzenoid Molecules	... Andrey A. Dobrynin and Ivan Gutman	845–856
Molecular Topology 22. ¹ Novel Connectivity Descriptors Based on Walk Degrees	... Mircea V. Diudea, Ovidiu M. Minailiuc, and Gabriel Katona	857–871
The Detour Index	... István Lukovits	873–882
Complexity of Some Interesting (Chemical) Graphs	... Sonja Nikolić, Nenad Trinajstić, Albin Jurić, Zlatko Mihalić, and Goran Krilov	883–897

(Continued on inside back cover)

(Continued from outside back cover)

Quantum Chemistry

- Development of a Quantum Chemical Two-Electron Integral Program for a Hierarchical Distributed Shared Memory Multiprocessor System (MEMSY)
... **Joachim Nedvidek and Peter Otto** 899–925
- Gram Detereminantal Inequalities with Elements $\langle r^m \rangle$ Obtained from Hylleraas Wave Functions for the 2S States of the Three-Electron Systems Li, Be⁺, B²⁺, C³⁺, N⁴⁺, O⁵⁺, F⁶⁺, and Ne⁷⁺ ... **P. Csavinszky** 927–932
- On the Definitions of Bond Index and Valence for Correlated Wave Functions
... **Robert Ponec, Filip Uhlik, David L. Cooper, and Karl Jug** 933–940
- Multicentre Bond Indices from the Generalized Population Analysis of Higher Order Densities ... **Robert Ponec and Filip Uhlik** 941–954
- The (– + –) Charge Distribution: A Common Pattern in the Transition State of Some Enzymes ... **Gábor Náray-Szabó and Timea Gérczei** 955–965

Synthesis & Spectroscopy

- New Acyclic Purine Nucleoside Analogues Containing Exocyclic Pyrrolo Moiety: Synthetic, NMR and X-ray Crystal Structure Studies ... **Silvana Raić, Mario Pongračić, Jasna Vorkapić Furač, Dražen Vikić-Topić, Antonija Hergold-Brundić, Ante Nagl, and Mladen Mintas** 967–986
- Merocyanine Isomers of *Spiro*[indolino-indolopyrans]: ¹H and ¹³C NMR and X-ray Crystal Structure Study ... **Silvana Raić, Jasna Vorkapić-Furač, Antonija Hergold-Brundić, Ante Nagl, Mladen Mintas, and Albrecht Mannschreck** 987–996
- Catalytic Intermediates in the Reaction of Deuterioferriheme with *m*-Chloroperoxybenzoic Acid ... **Vera Imper and Harold E. Van Wart** 997–1006
- Gas Phase Properties of ONOO-anion and ONOO-radical ... **Leo Klasinc, Dunja Srzić, Ljiljana Paša-Tolić, and Suzana Martinović** 1007–1011

Reflections

- On the Nature of Theoretical Research ... **Nenad Trinajstić** 1013–1022

The Fourth Croatian-Slovenian Crystallographic Meeting, Trakošćan 1995

- FOREWORD ... **B. Kamenar** XIII

(Continued on previous page)

The Home Page of Croat. Chem. Acta including all the Tables of Contents from 1996 may be found on the WWW under <http://pubwww.srce.hr/ccacaa>
Parts of the contents of *Croatica Chemica Acta* (e. g. figures or tables) may be reproduced without prior permission, provided reference is made to their source.

Photocopies of the articles are available through **The Genuine Article** ^(R) delivery program from:
Institute for Scientific Information
3501 Market Street
Philadelphia, PA 19104 USA

(Continued from inside back cover)

Structure of Molecules Assemblies	. . . István Hargittai and Magdolna Hargittai	1023–1038
Scanning Tunneling Microscopy of Surface Structures	. . . Velibor Marinković	1039–1052
Contributions of Crystallography to Materials Science	. . . Hartmut Fuess	1053–1067
Diffraction Line Broadening — Nuisance or Lattice-Imperfections Fingerprints	. . . Davor Balzar	1069–1115

Regular Scientific Papers

Physical and Theoretical Chemistry

Combinatorial Self-Similarity	. . . Sherif El-Basil	1117–1148
On the Counterion Adsorption Equilibrium	. . . Mihovil Hus	1149–1158
Estimation of the Normal Boiling Points of Haloalkanes Using Molecular Similarity	. . . Subhash C. Basak, Brian D. Gute, and Gregory D. Grunwald	1159–1173
A Correlation Rank Determinator for Principal Components	. . Damir Pavković, Vladislav Tomišić, Revik Nuss, and Vladimir Simeon	1175–1188
An Analysis of the Shape of the Coordination Polyhedron of Pentacoordinated Copper(II) Chelates with <i>N</i> -Alkylated Amino Acids	. . . Nenad Raos	1189–1200
UV Study of the Protonation of Indole and 3-Substituted Indoles in Perchloric Acid Media	. . . B. Andonovski, I. Spirevska, and A. Nikolovski	1201–1213

Inorganic Chemistry

Compensation Phenomena in β Relaxation of Novolac Phenol-Formaldehyde Resin. Influence of Water	. . . Mladen Topić and Zvonimir Katović	1215–1225
The Role of Oxygen Content in Electronic Structures of $\text{LaBa}_2\text{Cu}_3\text{O}_y$. . . Li Ming and Deng Chuanyue	1227–1238

Organic Chemistry

Synthesis of Some Pyridoxine and Pyridoxal Halophosphonates	. . . Sadik Elshani, Ljubica Butula, and Julija Matijević-Sosa	1239–1249
---	---	-----------

Analytical Chemistry

The Phase Composition of Electric Furnace Slag	. . . Štefica Cerjan-Stefanović, Alenka Rastovčan-Mioč, and Vjera Novosel-Radović	1251–1264
Evaluation and Selection of Optimal Solvent and Solvent Combinations in Thin-Layer Chromatography of Flavonoids and of Phenolic Acids of <i>Zizyphus juba</i> Mill	. . . Marica Medić-Šarić, Željko Maleš, Gordana Stanić, and Slavko Šarić	1265–1274

In Memoriam	A1–A2
Announcements and Advertisements	C9–C10