
**21th Dubrovnik International Course & Conference
MATH / CHEM / COMP 2006
Dubrovnik
June 19–24, 2006**

FOREWORD

Ante Graovac

Croat. Chem. Acta **80** (2007) XIX**Haruo Hosoya – Curriculum vitae**

Ante Graovac

Croat. Chem. Acta **80** (2007) XXI–XXII**ORIGINAL SCIENTIFIC PAPERS**

CCA-3153

On a Graph-Spectrum-Based Structure DescriptorIvan Gutman, Ernesto Estrada,
and Juan A. Rodríguez-Velázquez*Croat. Chem. Acta* **80** (2007) 151–154Let $\lambda_1, \lambda_2, \dots, \lambda_n$ be the eigenvalues of a (molecular) graph.

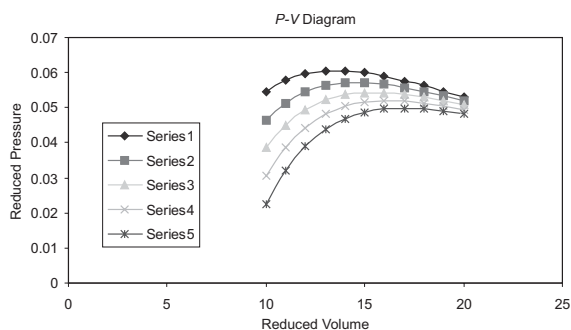
$$EE = \sum_{i=1}^n \exp(\lambda_i)$$

measures the 3D folding of long-chain molecules (*e.g.*, proteins) and the centrality of complex networks (such as neural, social, metabolic, or protein-protein interaction networks, as well as the Internet and the World Wide Web).

CCA-3154

Investigation of the Role of Coordination Number in the Lennard-Jones-Devonshire Theory

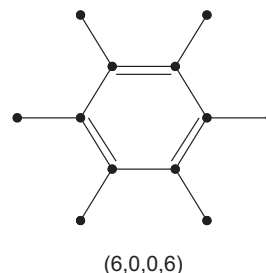
Gholamreza Vakili-Nezhaad

Croat. Chem. Acta **80** (2007) 155–158

CCA-3155

**Compact Valence Sequences for Molecules with Single, Double and Triple Covalent Bonds.
II. Graphs with Non-trivial Cycles**

Damir Vukičević and Ante Graovac

Croat. Chem. Acta **80** (2007) 159–164

CCA-3156

Comparing the Zagreb Indices

Pierre Hansen and Damir Vukičević

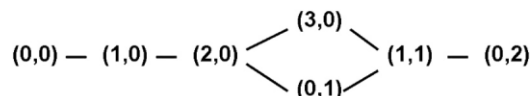
Croat. Chem. Acta **80** (2007) 165–168

$$\frac{\sum_{i \leq j} m_{ij} \cdot (i+j)}{\sum_{i \leq j} m_{ij} \cdot \left(\frac{1}{i} + \frac{1}{j}\right)} \leq \frac{\sum_{i \leq j \in N} m_{ij} \cdot i \cdot j}{\sum_{i \leq j \in N} m_{ij}}$$

CCA-3157

A Graph Theoretical Method for Partial Ordering of Alkanes

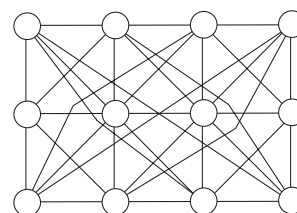
Damir Vukičević, Jelena Sedlar, and Sarah Michele Rajtmajer

Croat. Chem. Acta **80** (2007) 169–179

CCA-3158

K-dominating Sets on the Associative and Commutative Products of Two Paths

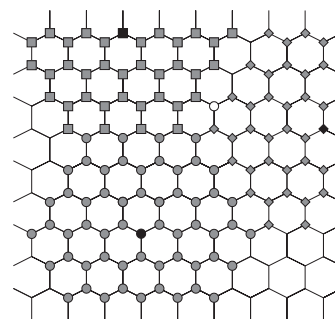
Antoaneta Klobučar

Croat. Chem. Acta **80** (2007) 181–185

CCA-3159

K-dominating Sets on Linear Benzenoids and on the Infinite Hexagonal Grid

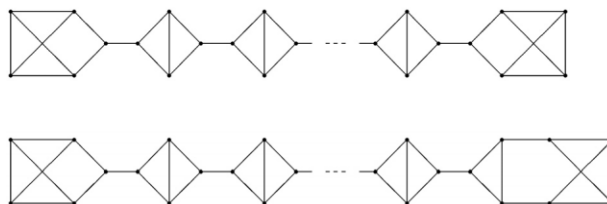
Damir Vukičević and Antoaneta Klobučar

Croat. Chem. Acta **80** (2007) 187–191

CCA-3160

Characterization of Trivalent Graphs with Minimal Eigenvalue Gap

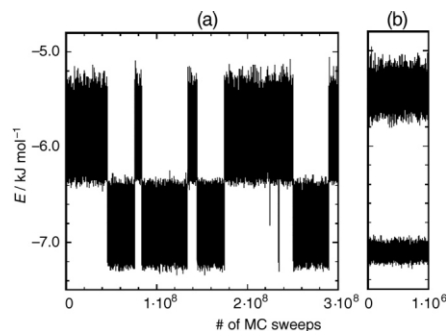
Clemens Brand, Barry Guiduli, and Wilfried Imrich

Croat. Chem. Acta **80** (2007) 193–201

CCA-3161

Multicanonical Monte Carlo Calculation of the First-order Phase Transition of Lennard-Jones Fluids

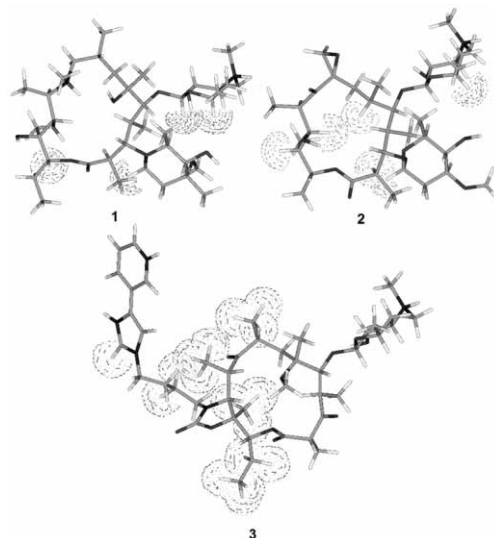
Chizuru Muguruma, Yuko Okamoto, and Masuhiro Mikami

Croat. Chem. Acta **80** (2007) 203–209

CCA-3162

Epitope Mapping of Macrolide Antibiotics to Bovine Serum Albumin by Saturation Transfer Difference NMR Spectroscopy

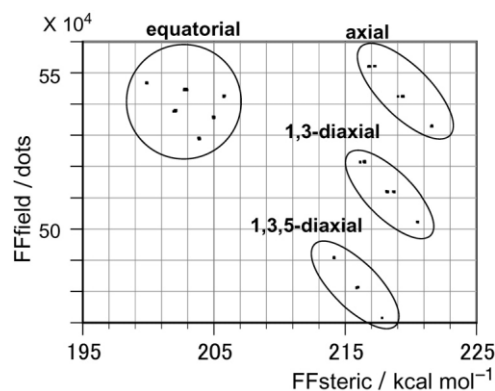
Predrag Novak, Predrag Tepeš, and Vedrana Lazić

*Croat. Chem. Acta* **80** (2007) 211–216

CCA-3163

Numerical Representation of Three-dimensional Stereochemical Environments Using FRAU-descriptors

Hiroko Satoh

*Croat. Chem. Acta* **80** (2007) 217–225

CCA-3164

Algebraic Characterization of Simple Transition-Metal Molecules

Ray Hefferlin and Ken Luk

$$C_1 + \sum_{i=0}^P v_{im} + 2 \sum_{j=0}^Q p_{jn} = R_1 \quad (0 \leq n \leq 1; 0 \leq m + n \leq 3)$$

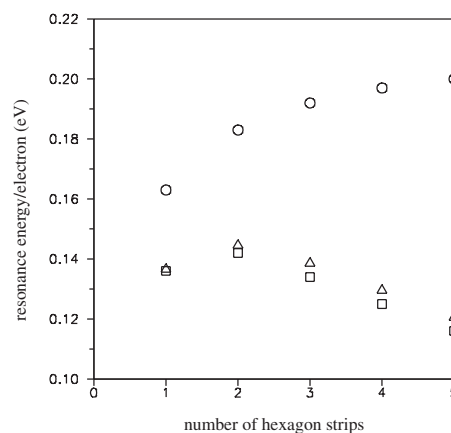
$$C_i + v_{im} = R_2 \quad (\text{if } m = 0 \text{ and } n = 0, \text{ then } C_k \rightarrow \text{Ne}; \text{ if } m = 0 \text{ and } n = 1, \text{ then } C_k \rightarrow \text{any entity that has bound-pair electrons})$$

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CCA-3165

Aromaticity of Carbon Nanotubes

István Lukovits, Franciska H. Kármán, Péter M. Nagy, and Erika Kálmán

*Croat. Chem. Acta* **80** (2007) 233–237

CCA-3166

Mathematical Meaning and Importance of the Topological Index Z

Haruo Hosoya

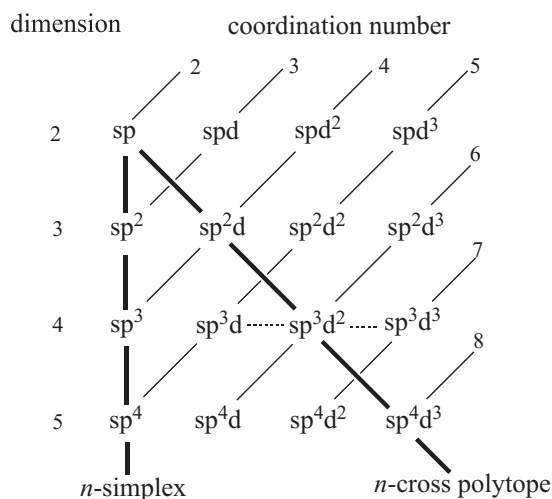
n	1	2	3	4	5	
S_n	•	••	•••	••••	•••••	F_n
	1	2	3	5	8	
U_n		□	□□	□□□	□□□□	P_n
	2	5	12	29	70	
V_n	∨	∨∨	∨∨∨	∨∨∨∨	∨∨∨∨∨	v_n
	3	10	33	109	360	
C_n	•	◊	△	□	◡	L_n
	1	3	4	7	11	
CU_n		◊	△	□	◡	Q_n
	2	6	14	34	82	
CV_n	∨	◊	△	□	◡	x_n
	3	11	36	119	393	

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CCA-3167

A New View of Hybridized Atomic Orbitals from N -dimensional World

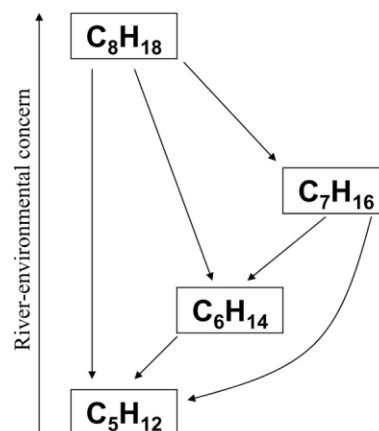
Haruo Hosoya, Fuyuko Kido, and Sumio Tokita

Croat. Chem. Acta **80** (2007) 251–260

CCA-3168

Partially Ordered Sets in the Analysis of Alkanes Fate in Rivers

Guillermo Restrepo, Rainer Brüggemann, and Kristina Voigt

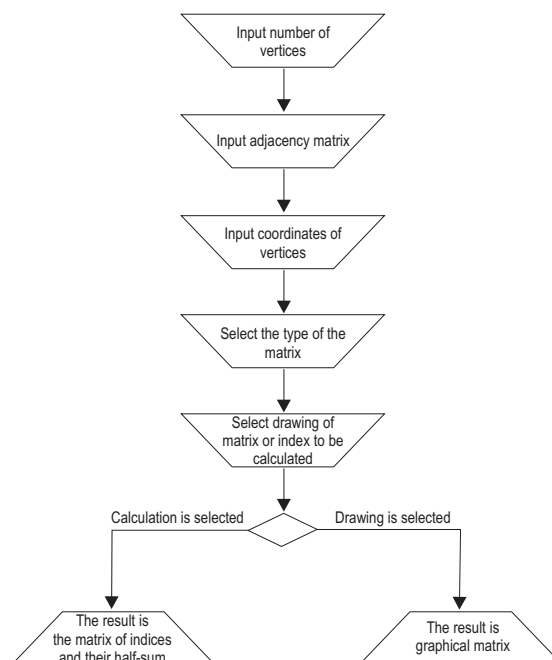
Croat. Chem. Acta **80** (2007) 261–270

CONFERENCE PAPERS

CCA-3169

**Hosoya Matrices as the Numerical Realization
of Graphical Matrices and Derived Structural
Descriptors**

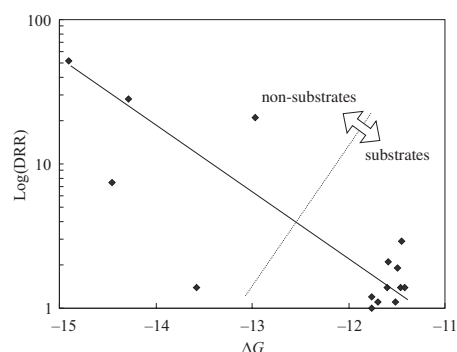
 Dušanka Janežič, Bono Lučić, Ante Miličević,
Sonja Nikolić, Nenad Trinajstić, and Damir Vukičević

Croat. Chem. Acta **80** (2007) 271–276


CCA-3170

**Theoretical Studies for Molecular Modeling
of New Camptothecin Analogues**

 Sachiko Aida-Hyugaji, Hiroshi Nakagawa,
Jumma Nomura, Minoru Sakurai, Umpei Nagashima,
and Toshihisa Ishikawa

Croat. Chem. Acta **80** (2007) 277–281


NOTE

CCA-3171

Altered Wiener Indices of Thorn Trees

Damir Vukičević, Bo Zhou, and Nenad Trinajstić

Croat. Chem. Acta **80** (2007) 283–285

$$W_{\min,k}(G) = \sum_{u,v \in E(G)} \left(n(G)^k m_G(u,v)^k - m_G(u,v)^{2k} \right)$$

APPENDIX

BOOK REVIEWS

Ivan Gutman	A23–A24
Nenad Trinajstić	A25–A26

OBITUARY

István Lukovits (1945–2007)	A27
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ANNOUNCEMENTS AND ADVERTISEMENTS

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**Proceedings of the
21th DUBROVNIK INTERNATIONAL COURSE & CONFERENCE
MATH / CHEM / COMP 2006**

Dubrovnik, June 19–24, 2006

Dedicated to Professor Haruo Hosoya on the occasion of his 70th birthday

Guest Editors:

**Ante Graovac, Biserka Pokrić,
and Dražen Vikić-Topić**

ZAGREB
CROATIA
2007