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A Contribution to the Celebration of the 100th Birth Anniversary of Professor Vladimir Prelog

EDITORIAL

Nikola Kallay, Predrag Novak, Bono Lučić, Greta Prajdić

Croat. Chem. Acta **79** (2006) XLVII

VLADIMIR PRELOG – Nobel Lecture

Croat. Chem. Acta **79** (2006) XLIX–LVII

20th Dubrovnik International Course & Conference
MATH / CHEM / COMP 2005
Dubrovnik
June 20–25, 2005

FOREWORD

Ante Graovac, Biserka Pokrić, and Dražen Vikić-Topić

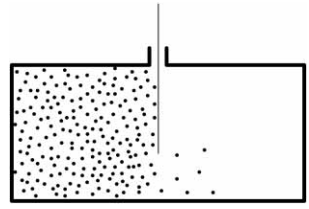
Croat. Chem. Acta **79** (2006) LXI

ORIGINAL SCIENTIFIC PAPERS

CCA-3098

Relaxation Processes, MaxEnt Formalism and Einstein's Formula for the Probability of Fluctuations

Paško Županović, Srećko Botrić, and Davor Juretić



Croat. Chem. Acta **79** (2006) 335–338

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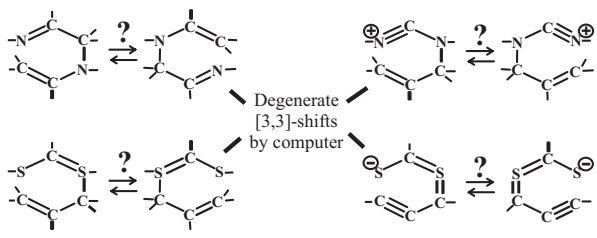
New Approaches to Degenerate Interconversions of Organic Structures: 1. Levels of Structural Degeneracy and Computer-aided Search for Degenerate Rearrangements

Serge S. Tratch, Marina S. Molchanova, and Nikolai S. Zefirov



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Generalized Operations on Maps

Mircea V. Diudea, Monica Stefu, Peter E. John, and Ante Graovac

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Generalized Polansky Index as an Aromaticity Measure in Polycyclic Aromatic Hydrocarbons

Patrick Bultinck, Robert Ponec, Ana Gallegos, Stijn Fias, Sofie Van Damme, and Ramon Carbó-Dorca

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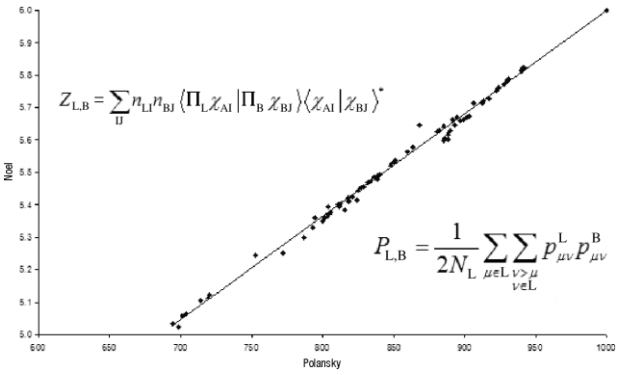
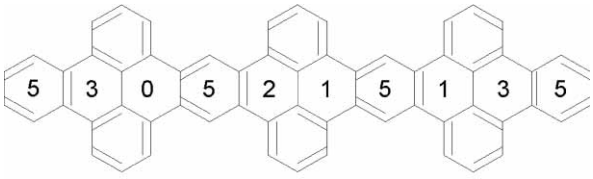


CCA-3102

On Algebraic and Geometric Kekulé Structures in Benzenoid Rotagraphs

Ante Graovac, Damir Vukičević, and Janez Žerovnik

Croat. Chem. Acta **79** (2006) 373–377



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Alpha-melanotropin Peptide: Structure and Ligand–Receptor Recognition

Karlo Houra, Nikola Štambuk, Paško Konjevoda, Alenka Boban-Blagaić, Tomislav Bruketa, and Biserka Pokrić

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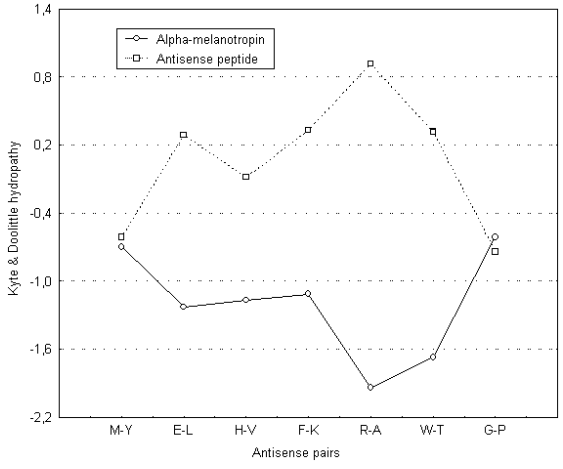

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Modelling of Convective Carrot Drying

Damir Ježek, Branko Tripalo, Mladen Brnčić, Damir Karlović, Dražen Vikić-Topić, and Zoran Herceg

Croat. Chem. Acta **79** (2006) 385–391

$$X(t) = X_0 e^{-bt^{-d}} \quad (1)$$

$$(-\mathrm{d}X/\mathrm{d}t) = b \cdot d \cdot t^{(d-1)} \cdot X(t) \quad (2)$$

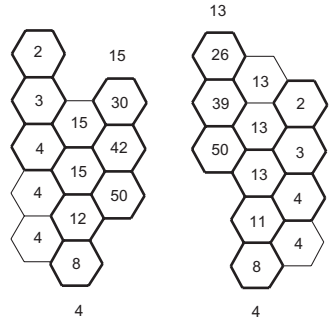
$$S(a,b,d) = \sum_{i=1}^{n} (X_0 - X_{\mathrm{eq}}) \cdot \exp(-b \cdot t^d) - X_{\mathrm{eq}}) - X_i)^2 \quad (3)$$

CCA-3105

Enumeration of Kekulé Structures in Defective Patterns of Rectangular Graphite

István Lukovits

Croat. Chem. Acta **79** (2006) 393–397



CCA-3106

The Metric Index

Matevž Bren and Vladimir Batagelj

Croat. Chem. Acta **79** (2006) 399–410

Some well-known similarities

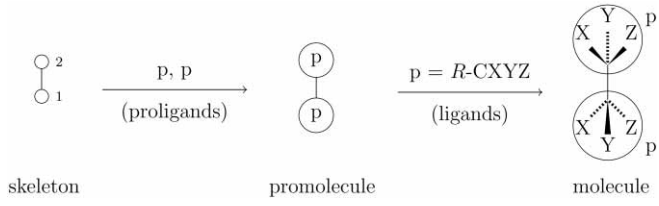
	Definition	θ	p
Kendall, Sokal-Michener (1958)	$\frac{a+d}{m}$	S_1	1
Rogers & Tanimoto (1960)	$\frac{a+d}{a+d+2(b+c)}$	S_2	$\frac{\log\frac{2}{3}}{\log\frac{1}{2}} = 1.709$
Jaccard (1900)	$\frac{a}{a+b+c}$	T_1	1
Dice (1945), Czekanowski (1913)	$\frac{a}{a+\frac{1}{2}(b+c)}$	$T_{1/2}$	$\frac{\log 2}{\log 3} = 0.630$
Sokal & Sneath	$\frac{a}{a+2(b+c)}$	T_2	$\frac{\log\frac{2}{3}}{\log\frac{1}{2}} = 1.709$

CCA-3107

Sphericities of Cycles. What Pólya's Theorem is Deficient in for Stereoisomer Enumeration

Shinsaku Fujita

Croat. Chem. Acta **79** (2006) 411–427



CCA-3108

On Instability of Fullerene C_{72}

Damir Vukičević, Ivan Gutman, and Milan Randić

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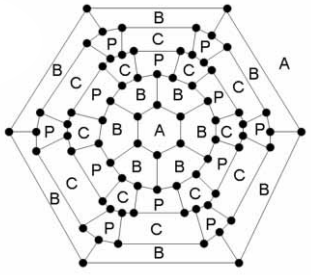

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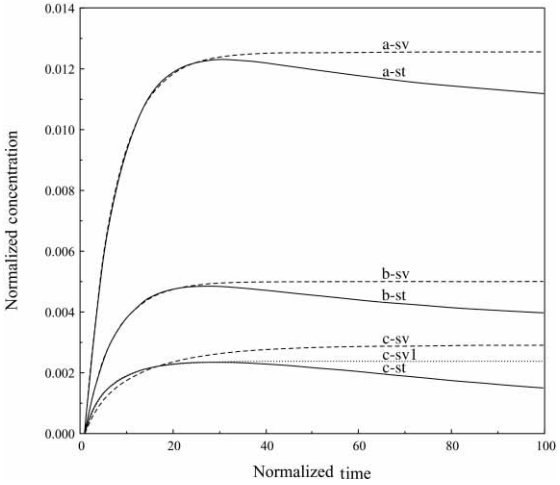
Reaction Kinetics in Intracellular Environments: The Two Proposed Models Yield Qualitatively Different Predictions

Željko Bajzer, Miljenko Huzak, Kevin Neff, and Franklyn G. Prendergast

Croat. Chem. Acta **79** (2006) 437–444



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Omega Polynomial in Tubular Nanostructures

Mircea V. Diudea, Simona Cigher, Aniela E. Vizitiu, Oleg Ursu, and Peter E. John

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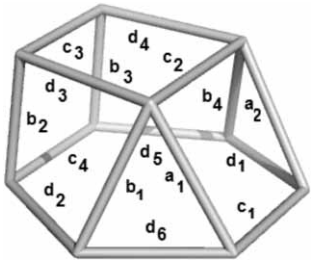

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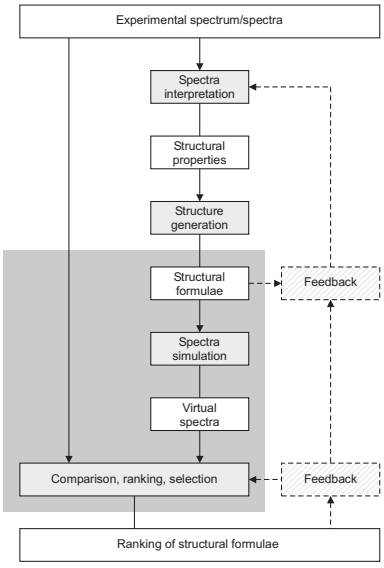
CASE via MS: Ranking Structure Candidates by Mass Spectra

Adalbert Kerber, Markus Meringer, and Christoph Rücker

Croat. Chem. Acta **79** (2006) 449–464



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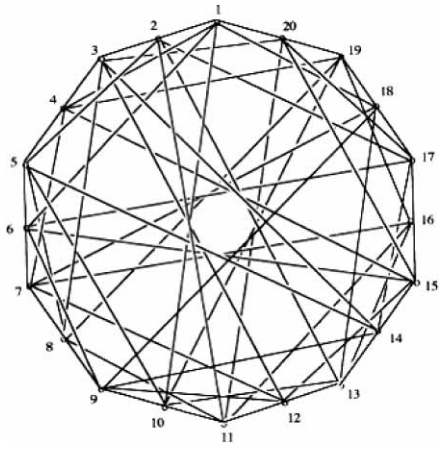
On Symmetry of Some Non-transitive Chemical Graphs

Gorban Ali Moghani and Ali Reza Ashrafi

Croat. Chem. Acta **79** (2006) 465–469



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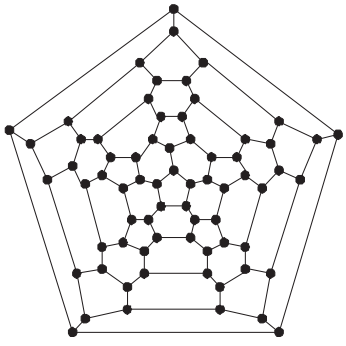
Kekulé Structures of Fullerene C_{70}

Milan Randić and Damir Vukičević

Croat. Chem. Acta **79** (2006) 471–481



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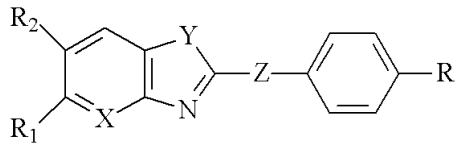
QSAR Modeling of Antifungal Activity of Some Heterocyclic Compounds

Oleg Ursu, Adina Costescu, Mircea V. Diudea, and Bazil Parv

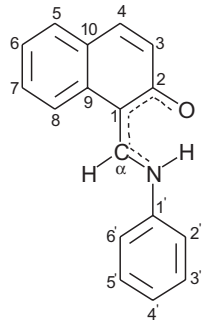


Croat. Chem. Acta **79** (2006) 483–488

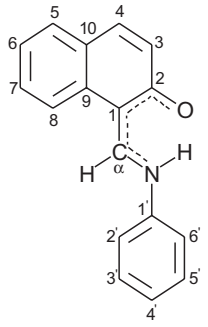
CCA-3115

NMR Spectroscopy of 2-Hydroxy-1-naphthylidene Schiff Bases with Chloro and Hydroxy Substituted Aniline Moiety

Julija Matijević-Sosa, Marijana Vinković, and Dražen Vikić-Topić



1, 2 ($OH_{2'}$), 4, 5 ($OH_{2'}$), 6



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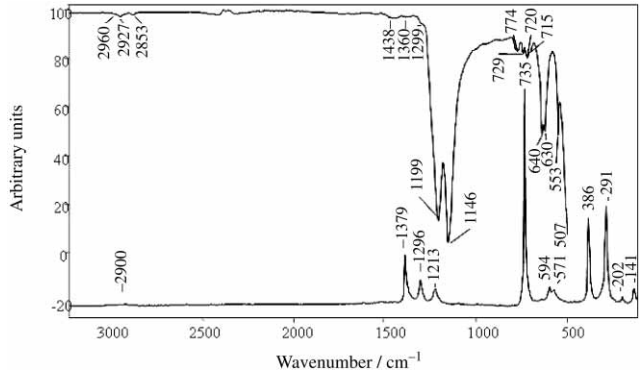
FTIR and FT-Raman Spectroscopic Study on Polymer Based High Pressure Digestion Vessels

Judith Mihály, Silvana Sterkel, Hugo M. Ortner, László Kocsis, László Hajba, Éva Furdyga, and János Mink



Croat. Chem. Acta **79** (2006) 497–501

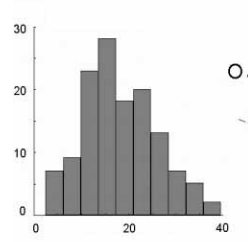
CONFERENCE PAPER

CCA-3117

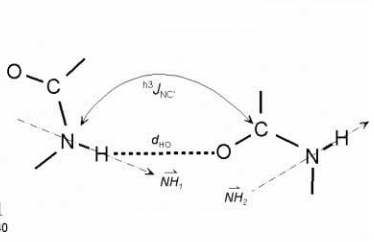
NMR $^{h3}J_{NC'}$ Couplings Provide Comprehensive Geometrical Constraints for Protein H-bonds in Solution

Nenad Juranić, Martin C. Moncrieffe, Elena Atanasova, Slobodan Macura, and Franklyn G. Prendergast

$\Delta\alpha_{NH_NH} = 20° \pm 10° \quad \Leftrightarrow \quad |^{h3}J_{NC'}| > 0.3$ Hz



$\Delta\alpha_{NH_NH}$



$\sphericalangle(N\vec{H}_1, N\vec{H}_2) = \Delta\alpha_{NH_NH}$

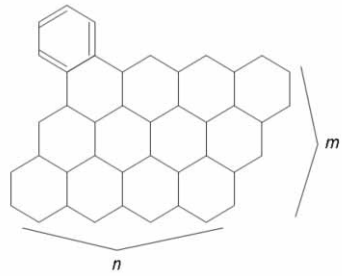
Croat. Chem. Acta **79** (2006) 503–507

NOTE

CCA-3118

Counting Kekulé Structures of Benzenoid Parallelograms Containing One Additional Benzene Ring

Damir Vukičević, István Lukovits, and Nenad Trinajstić



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APPENDIX

BOOK REVIEW

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ANNOUNCEMENTS AND ADVERTISEMENTS A33