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Sonja Nikolić

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Sonja Nikolić

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Nenad Trinajstić – Pioneer of Chemical Graph Theory

Milan Randić

Beginnings of Chemical Graph Theory

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REVIEW

CCA-2897

Shedding Light on Light

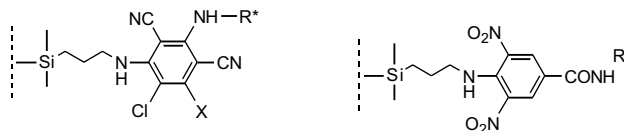
John Murrell

Let there be light...

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**Experiments and Models in Enantiorecognition
by Chiral Pirkle-type Stationary Phases
Containing Aromatic π -Acid Branching Units**
Darko Kontrec, Vladimir Vinković, Maja Šepelj,
and Vitomir Šunjić

X = Cl, R* = chiral selector ← branch-type CSPs → R* = chiral selector
X = NH-R* ← tweezer-type CSPs

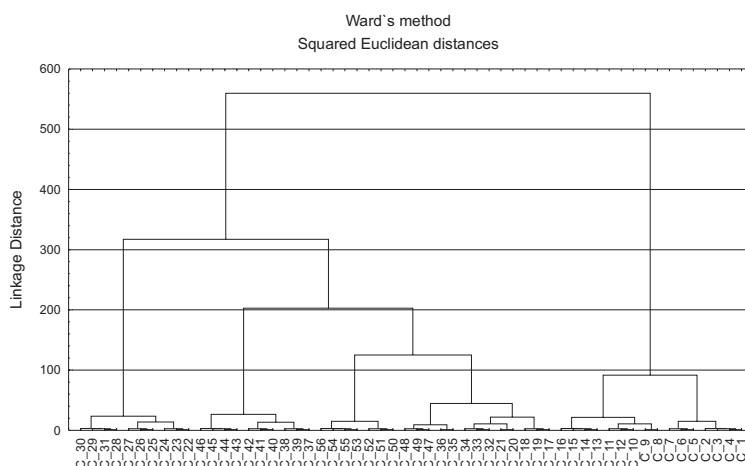
Croat. Chem. Acta **77** (2004) 31–51

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**Application of Cluster Analysis in Search
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by the Overlapping Spheres Method**

Nenad Raos and Lora Žuža-Mak

*Croat. Chem. Acta* **77** (2004) 53–60

CCA-2900

A New Hyper-Wiener Index

Ivan Gutman

$$W = \sum_e n_1(e,e) n_2(e,e)$$

$$WW = \sum_{e,f} n_1(e,f) n_2(e,f)$$

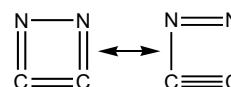
$$WWW = \sum_{e,f} n_0(e,f) n_1(e,f) n_2(e,f)$$

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CCA-2901

**Global Molecular Identification from Graphs. IV.
Molecules with Four Closed p-Shell Atoms and beyond**

Chris J. Walters, Ken Caviness, and Ray A. Hefferlin

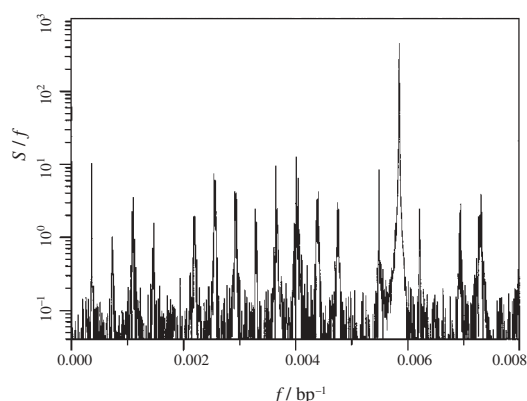
*Croat. Chem. Acta* **77** (2004) 65–71*Croat. Chem. Acta* **77** (1–2) V–XV (2004)

CCA-2902

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Croat. Chem. Acta **77** (2004) 73–81

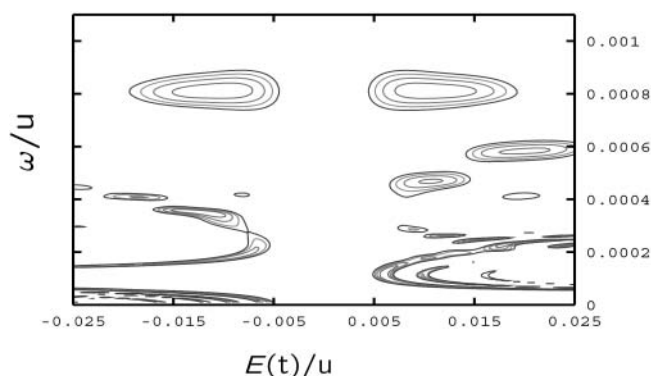


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On the Robustness of Low-frequency Laser Control Schemes for Proton Transfer in Thioacetylacetone

Iva Tatić and Nađa Došlić

Croat. Chem. Acta **77** (2004) 83–88

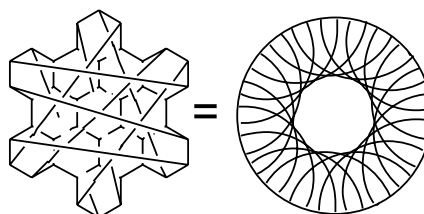


CCA-2904

Supersymmetry of Hexabenzocoronene Torus

Haruo Hosoya, Yoko Tsukano, Kyoko Nakada,
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CCA-2905

On Variable Zagreb Indices

Ante Miličević and Sonja Nikolić

Croat. Chem. Acta **77** (2004) 97–101

$${}^vM_1 = \sum_{\text{vertices}} [d(i) d(i)]^\lambda$$

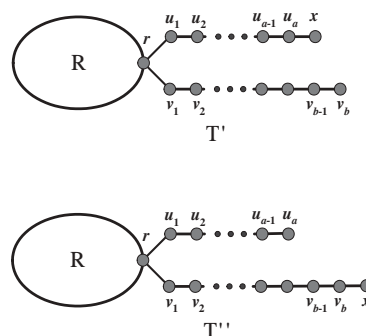
$${}^vM_2 = \sum_{\text{edges}} [d(i) d(j)]^\lambda$$

CCA-2906

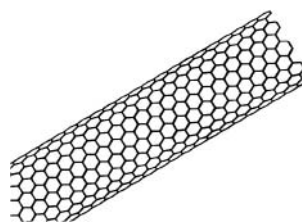
A Class of Modified Wiener Indices

Ivan Gutman, Damir Vukičević, and Janez Žerovnik

Croat. Chem. Acta **77** (2004) 103–109



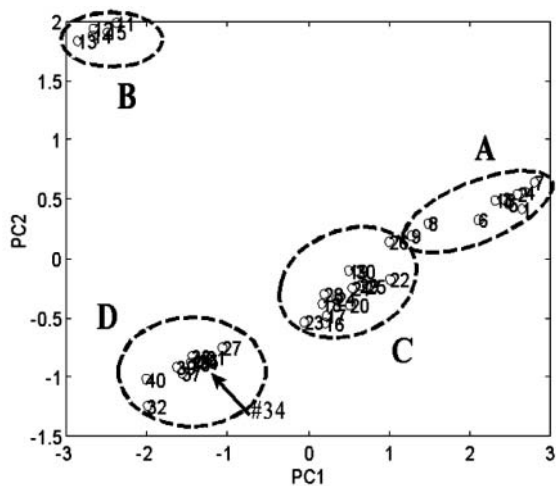
CCA-2907

Wiener Index of Armchair Polyhex NanotubesMircea V. Diudea, Monica Stefu, Basil Pârv,
and Peter E. John*Croat. Chem. Acta* **77** (2004) 111–115An »armchair« TUV $C_6[20,n]$

CCA-2908

**Procrustes Rotation and Pair-wise Correlation:
a Parametric and a Non-parametric Method
for Variable Selection**

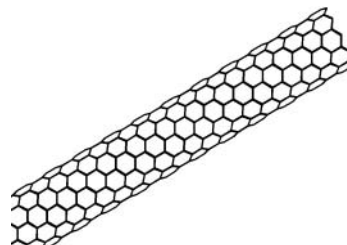
Károly Héberger and José M. Andrade

Croat. Chem. Acta **77** (2004) 117–125

CCA-2909

Wiener Index of Zig-zag Polyhex Nanotubes

Peter E. John and Mircea V. Diudea

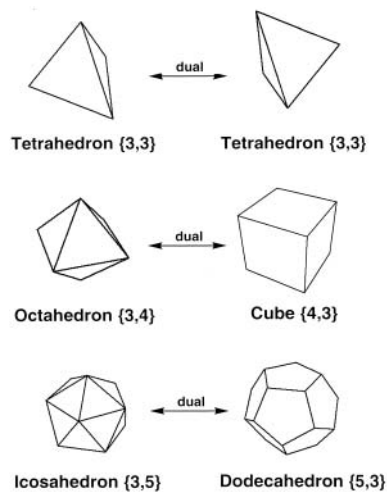
Croat. Chem. Acta **77** (2004) 127–132

A »zig-zag« polyhex nanotube

CCA-2910

Regular Polytopes, Root Lattices, and Quasicrystals

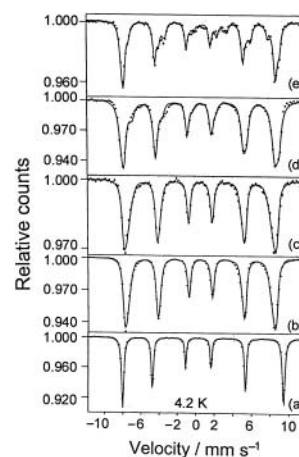
R. Bruce King

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The Effect of Bicarbonate/Carbonate Ions on the Formation of Iron Rust

Svetozar Musić, Israel Nowik, Mira Ristić, Zvonko Orehovec, and Stanko Popović

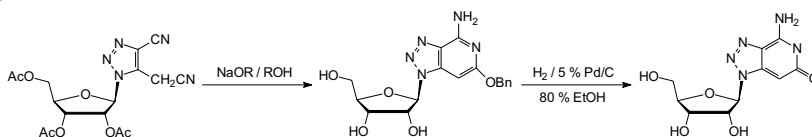


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Synthesis of 8-Aza-3-deazaisoguanosine by a Novel Ring Closure of Dinitriles by Sodium Alkoxides

Marjan Ješelnik, Suzana Jakša, and Jože Kobe

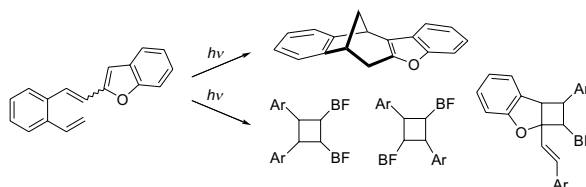


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Irena Škorić, Željko Marinić, and Marija Šindler-Kulyk

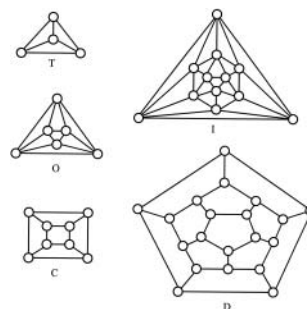


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CCA-2914

On the Complexity of Platonic Solids

Danail Bonchev

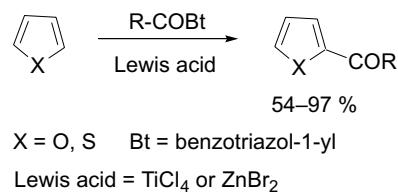


Croat. Chem. Acta **77** (2004) 167–173

CCA-2915

C-Acylation of 2-Methylfuran and Thiophene using *N*-Acylobenzotriazoles

Alan R. Katritzky, Kazuyuki Suzuki, and Sandeep K. Singh

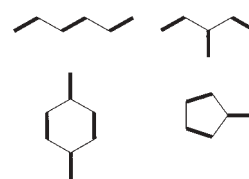


Croat. Chem. Acta **77** (2004) 175–178

CCA-2916

Minimally Kekulenoid π -Networks and Reactivity for Acyclic

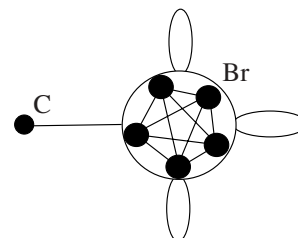
Douglas J. Klein and Anirban Misra

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CCA-2917

Modeling with Indices Obtained from Complete Graphs

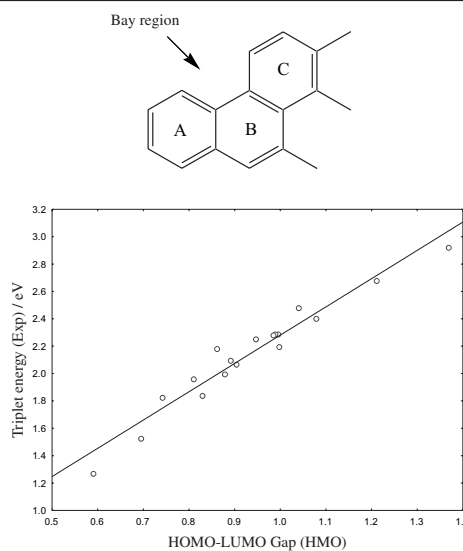
Lionello Pogliani

Croat. Chem. Acta **77** (2004) 193–201

CCA-2918

On the Usefulness of Graph-theoretic Descriptors in Predicting Theoretical Parameters. Phototoxicity of Polycyclic Aromatic Hydrocarbons (PAHs)

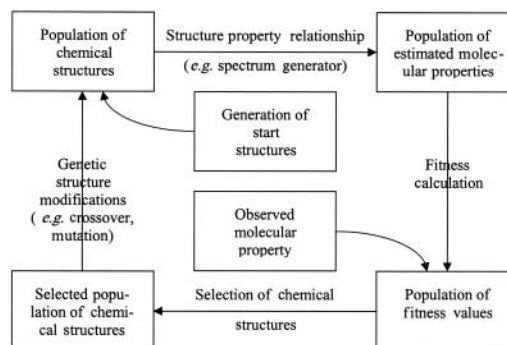
Ernesto Estrada and Grace Patlewicz

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Application of Genetic Algorithms to Structure Elucidation of Halogenated Alkanes Considering the Corresponding ^{13}C NMR Spectra

Thomas Blenkins and Peter Zinn

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In Search of Simplification: the Use of Topological Complexity Indices to Guide Retrosynthetic Analysis

Steven H. Bertz and Christoph Rücker

Croat. Chem. Acta **77** (2004) 221–235

$$\Delta C(\text{reaction}) = C(\text{products}) - C(\text{reactants}) \quad (1)$$

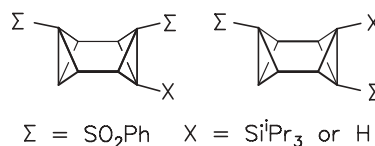
$$\Delta C(\text{transform}) = C(\text{precursors}) - C(\text{target}) \quad (2)$$

$$\Delta C(\text{transform}) = -\Delta C(\text{reaction}) \quad (3)$$

CCA-2921

***E/Z* Isomerism Without a Double Bond – an Unusual Type of Stereoisomerism, and an Unprecedented Isomerisation in a Bicyclobutane**

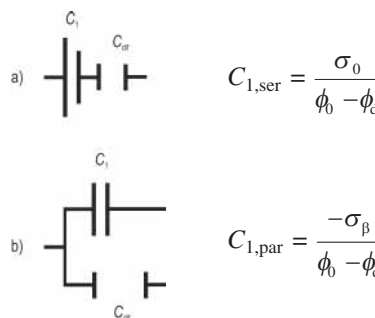
Christoph Rücker and Gunter Haftstein

*Croat. Chem. Acta* **77** (2004) 237–241

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Inner Layer Capacitor at the Solid/Liquid Interface

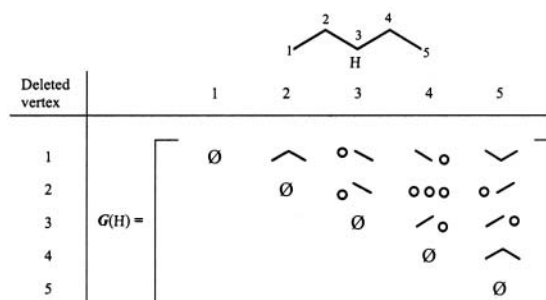
Nikola Kallay, Davor Kovačević, Ana Čop, and Martina Medvidović

*Croat. Chem. Acta* **77** (2004) 243–249

CCA-2923

Novel Graphical Matrix and Distance-based Molecular Descriptors

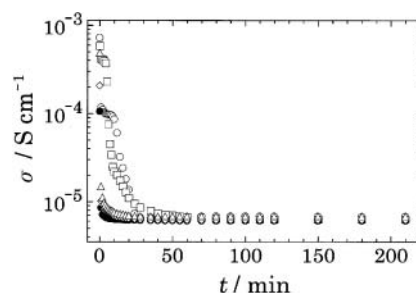
Milan Randić, Nabamita Basak, and Dejan Plavšić

*Croat. Chem. Acta* **77** (2004) 251–257

CCA-2924

Time and Composition Dependent Electrical Conductivity of Vanadate Glasses Showing Both Cationic Conduction and Electronic Conduction

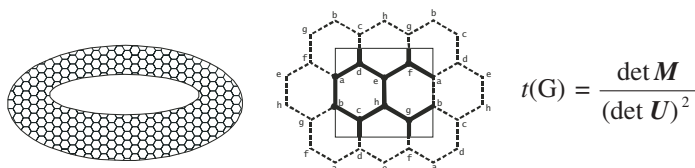
Atsushi Ikeda, Ken-ichi Fukuda, and Tetsuaki Nishida

*Croat. Chem. Acta* **77** (2004) 259–262

CCA-2925

A Theorem for Counting Spanning Trees in General Chemical Graphs and Its Particular Application to Toroidal Fullerenes

Edward C. Kirby, Douglas J. Klein, Roger B. Mallion, Paul Pollak, and Horst Sachs

*Croat. Chem. Acta* **77** (2004) 263–278

CCA-2926

**On the Interaction of an Isolated State
with the Known Infinite-dimensional
Quantum System**

Tomislav P. Živković

Croat. Chem. Acta 77 (2004) 279–293

$$f(\varepsilon) = \sum_{\nu} f_{\nu}(\varepsilon), \quad \omega(\varepsilon) = \sum_{\nu} \omega_{\nu}(\varepsilon), \quad \omega_{\nu}(\varepsilon) = P \int \frac{f_{\nu}(\lambda)}{\varepsilon - \lambda} d\lambda.$$

$$\beta^2 \omega(\varepsilon_I) + E - \varepsilon_I = 0, \quad w_I^a = \frac{1}{1 - \beta^2 \omega^{(1)}(\varepsilon_I)}, \quad \varepsilon_I \notin D.$$

$$\rho^a(\varepsilon) = \frac{\beta^2 f(\varepsilon)}{\pi^2 \beta^4 f(\varepsilon)^2 + (\beta^2 \omega(\varepsilon) + E - \varepsilon)^2}, \quad \varepsilon \in D.$$

$$\rho_{\nu}^b(\lambda, t) = |u_{\nu}^b(\lambda, t)|^2, \quad \lambda \in I_{\nu}.$$

$$u_{\nu}^b(\lambda, t) = \beta \sqrt{f_{\nu}(\lambda)} \left[\int \frac{\rho^a(\varepsilon) [e^{-i(\varepsilon-\lambda)t/\hbar} - 1]}{\varepsilon - \lambda} d\varepsilon + \sum_I w_I^a \frac{[e^{-i(\varepsilon_I-\lambda)t/\hbar} - 1]}{\varepsilon_I - \lambda} \right].$$

CCA-2927

**Constructive Enumeration of Chiral Isomers
of Alkanes**

István Lukovits

Croat. Chem. Acta 77 (2004) 295–300

Theorem 1.

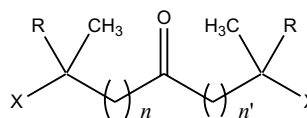
Of all possible MTs related to the same tree, T, the LDF (or canonically numbered) tree will have the minimal valence code and the maximal CAM.

CCA-2928

**Lipophilicity Parameters and Biological Activity
in a Series of Compounds
with Potential Cardiovascular Applications**

Emil Pop, Daniela C. Oniciu, Michael E. Pape,
Clay T. Cramer, and Jean-Louis H. Dasseux

Croat. Chem. Acta 77 (2004) 301–306



CCA-2929

Oxidation-induced Spin Probes in Low-density Lipoproteins

Dubravka Krilov, Marta Žuvić-Butorac, Nataša Stojanović,
and Janko N. Herak

Croat. Chem. Acta 77 (2004) 307–311

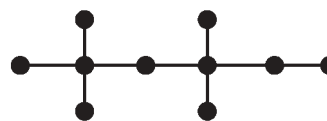


CCA-2930

**On Molecular Graphs with Valencies
1, 2 and 4 with Prescribed Numbers of Bonds**

Damir Vukičević and Ante Graovac

Croat. Chem. Acta 77 (2004) 313–319



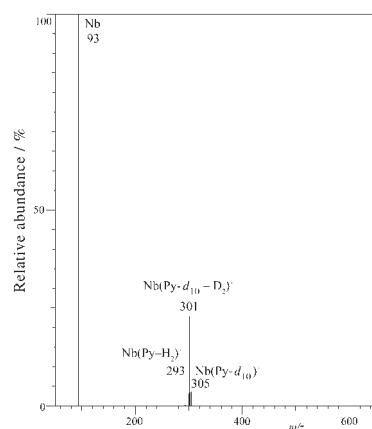
$$m_{11} = 0, m_{12} = 1, m_{14} = 5,$$

$$m_{22} = 0, m_{24} = 3, m_{44} = 0$$

CCA-2931

Isotope Effect in the Gas Phase Reaction of Pyrene- d_{10} with Nb^+ Ions

Saša Kazazić, Leo Klasinc, Marko Rožman, Dunja Srzić, and Jan von Knop

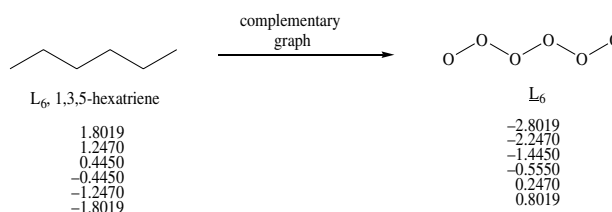


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CCA-2932

Properties and Relationships of Conjugated Polyenes Having a Reciprocal Eigenvalue Spectrum – Dendralene and Radialene Hydrocarbons

Jerry Ray Dias

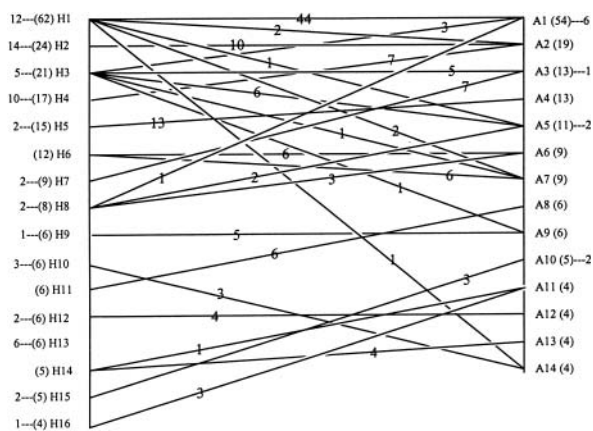


Croat. Chem. Acta **77** (2004) 325–330

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Interrelationship of Major Topological Indices Evidenced by Clustering

Subhash C. Basak, Brian D. Gute, and Alexandru T. Balaban

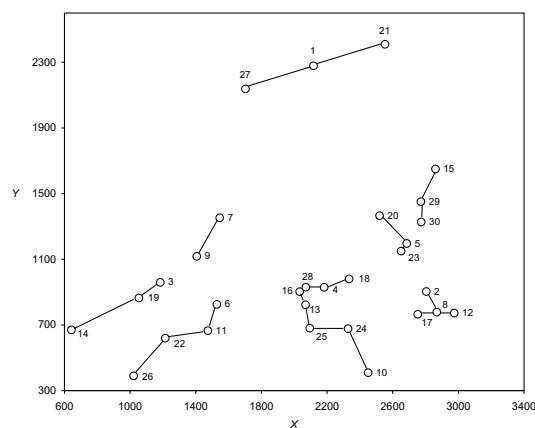


Croat. Chem. Acta **77** (2004) 331–344

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Characterization of 2-D Proteome Maps Based on the Nearest Neighborhoods of Spots

Milan Randić, Nella Lerš, Dejan Plavšić, and Subhash C. Basak

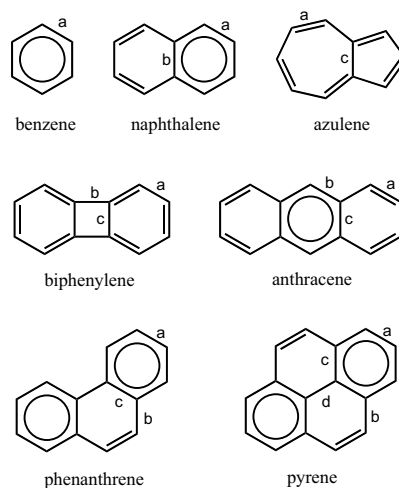


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CCA-2935

Partly Olefinic Reference Structure Defined to Evaluate Bond Resonance Energy and the Ring Current It Would Sustain

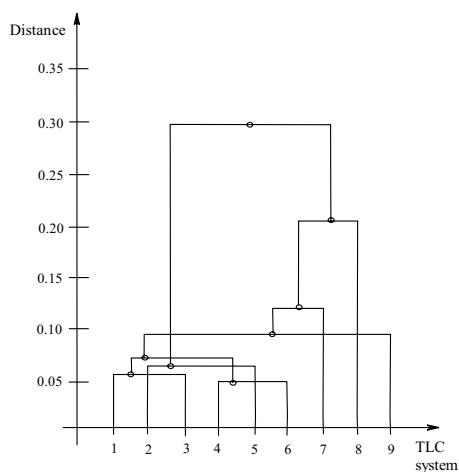
Jun-ichi Aihara, Rika Sekine, and Sumio Oe

*Croat. Chem. Acta* **77** (2004) 353–359

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Optimization of Chromatographic Conditions in Thin Layer Chromatography of Flavonoids and Phenolic Acids

Marica Medić-Šarić, Ivona Jasprica, Asja Smolčić-Bubalo, and Ana Mornar

*Croat. Chem. Acta* **77** (2004) 361–366

CCA-2937

Experimental and Calculation Procedures for Molecular Lipophilicity: A Comparative Study for 3,3'-(2-Methoxybenzylidene)-bis(4-hydroxycoumarin)

Marica Medić-Šarić, Ana Mornar, Tanja Badovinac-Črnjević, and Ivona Jasprica

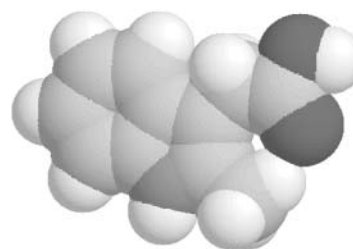
	log <i>P</i>	$\Delta(\log P_{\text{est.}} - \log P_{\text{exp.}})$
»shake-flask«	2.5	/
HyperChem 7.0	2.54	0.04
XLOGP	4.54	2.04
LogKow	3.64	1.14
CLOGP	4.32	1.82
ALOGPS 2.1	3.06	0.56
IA logP	4.11	1.61

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Ab initio Hartree-Fock Investigation of 2-Methylindole-3-acetic Acid

Michael Ramek and Sanja Tomić

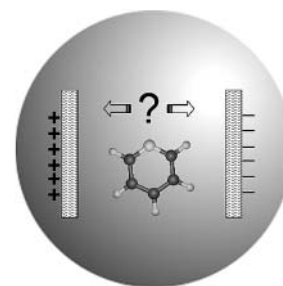
*Croat. Chem. Acta* **77** (2004) 371–376

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Categorical Modeling of the Flow Pattern of Liquid Organic Compounds Between Blade Electrodes Using Semiempirical and *ab initio* Quantum Chemical Descriptors

Takahiro Suzuki, Kohei Yoshida, Hiroya Onizuka, Yoshio Iwai, Yasuhiko Arai, Aynur Aptula, Ralph Kühne, Ralf-Uwe Ebert, and Gerrit Schüürmann

Croat. Chem. Acta **77** (2004) 377–389



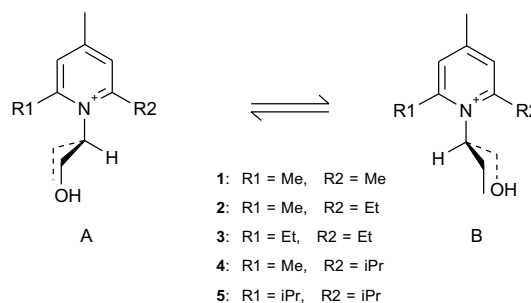
Prediction by QSAR

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Rotation Barriers in Pyridinium Salts Depend on the Number of Available Ground State Conformations

Ion Ghiviriga, Edmund W. Czerwinski, and Alexandru T. Balaban

Croat. Chem. Acta **77** (2004) 391–396

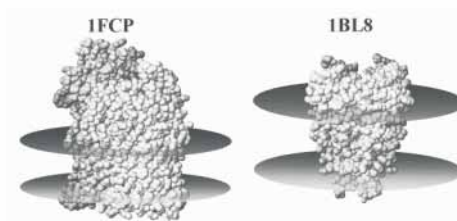


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Precise Annotation of Transmembrane Segments with Garlic – a Free Molecular Visualization Program

Damir Zucić and Davor Juretić

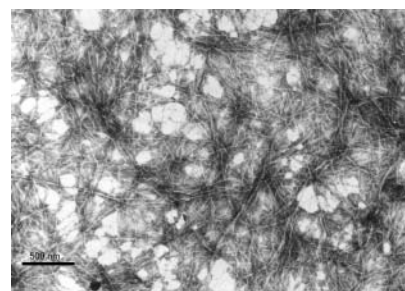
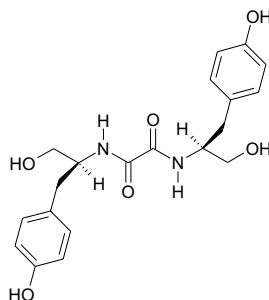
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CCA-2942

Chiral Bis(tyrosinol) and Bis(*p*-hydroxyphenylglycinol) Oxalamide Gelators. Influence of Aromatic Groups and Hydrogen Bonding on Gelation Properties

Janja Makarević, Milan Jokić, Zlata Raza, Vesna Čaplar, Darinka Katalenić, Zoran Štefanić, Biserka Kojić-Prodić, and Mladen Žinić



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APPENDIX

INSTRUCTIONS TO AUTHORS

A1–A4

ANNOUNCEMENTS AND ADVERTISEMENTS

A5–A8