

INTRODUCTION

FOREWORD

Bono Lučić, Hrvoj Vančik and Jerzy Ciośłowski, Olga Kronja

Croat. Chem. Acta 2020, 93(4), 245–245

REMINISCENCE

My Tortuous Pathway Through Mathematical Chemistry and QSAR Research With Memories of Some Personal Interactions and Collaborations With Professors Milan Randić and Mircea Diudea

Subhash C. Basak

Croat. Chem. Acta 2020, 93(4), 247–258

DOI: 10.5562/cca3759

REMINISCENCE

Reminiscences of Milan Randić

Roger Mallion

Croat. Chem. Acta 2020, 93(4), 259–260

DOI: 10.5562/cca3787

SCIENTIFIC ARTICLES

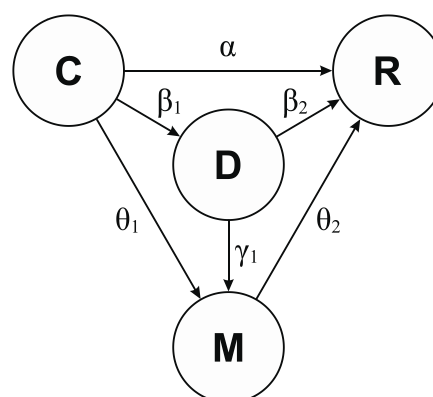
REVIEW

Applications of Multidimensional Space of Mathematical Molecular Descriptors in Large-Scale Bioactivity and Toxicity Prediction- Applications to Prediction of Mutagenicity and Blood-Brain Barrier Entry of Chemicals

Subhash C. Basak, Subhabrata Majumdar, Claudiu Lungu

Croat. Chem. Acta 2020, 93(4), 261–272

DOI: 10.5562/cca3772



Some Less Familiar Properties of Randić Index

Ivan Gutman

Croat. Chem. Acta **2020**, 93(4), 273–278

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$$R(G) = \frac{n}{2} - \sum_{ij \in E(G)} \left(\frac{1}{\sqrt{d_i}} - \frac{1}{\sqrt{d_j}} \right)^2$$

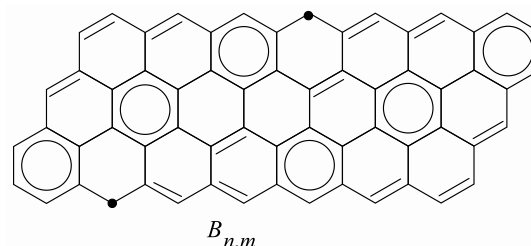
$$\Rightarrow \begin{cases} \min R(T_n) = R(P_n) \\ \max R(T_n) = R(S_n) \end{cases}$$

Computing Degeneracies of the Most Important Structures of Polycyclic Aromatic Hydrocarbons

Tomislav Došlić

Croat. Chem. Acta **2020**, 93(4), 279–287

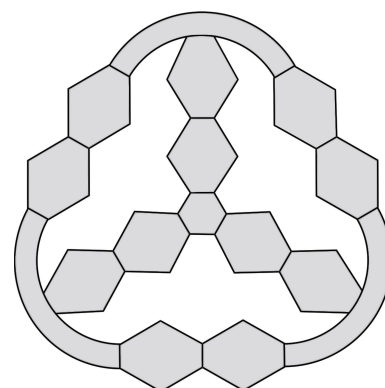
DOI: 10.5562/cca3752

**Catacondensed Chemical Hexagonal Complexes: A Natural Generalisation of Benzenoids**

Cate S. Anstöter, Nino Bašić, Patrick W. Fowler, Tomaž Pisanski

Croat. Chem. Acta **2020**, 93(4), 289–301

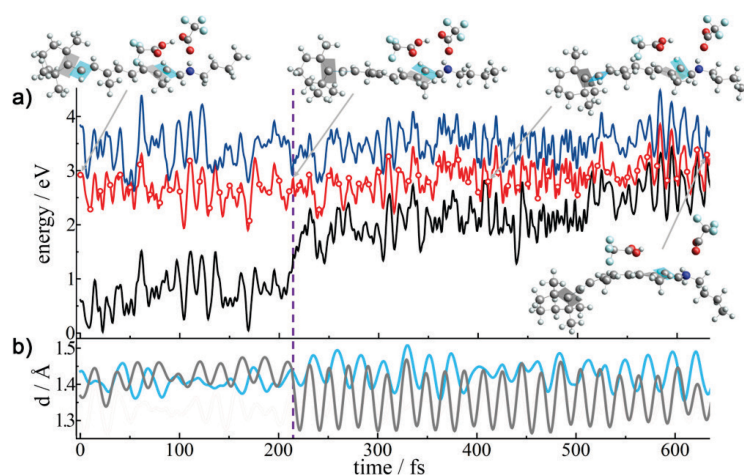
DOI: 10.5562/cca3765

**On the Possible Role of an Intermolecular Charge Transfer State in the Excitation of the Biologically Active Bond of the Retinal Chromophore-counterion Pair**

Jurica Novak, Momir Mališ, Nađa Došlić

Croat. Chem. Acta **2020**, 93(4), 303–310

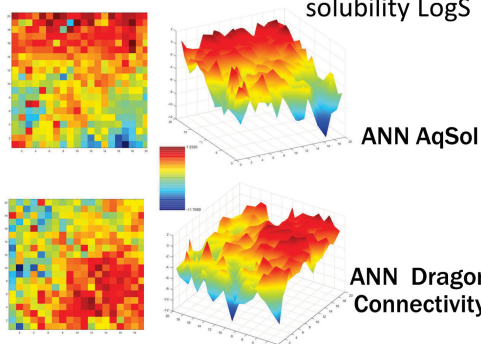
DOI: 10.5562/cca3748



QSPR Models for Prediction of Aqueous Solubility: Exploring the Potency of Randić-type Indices

Janja Sluga, Katja Venko, Viktor Drgan, Marjana Novič

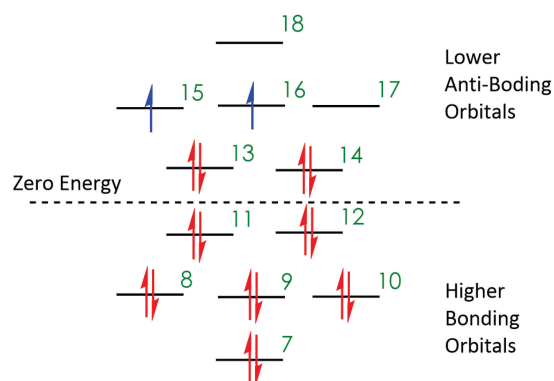
Response surface of CP-ANN models of
solubility LogS



Croat. Chem. Acta **2020**, 93(4), 311–319
DOI: 10.5562/cca3776

Postscript on Viable Ground-States for Calculating Topological π -Electron Ring-Currents Using the Hückel–London–Pople–McWeeny Model

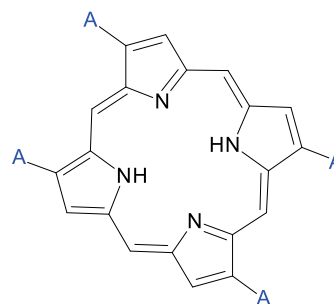
Timothy K. Dickens, Roger B. Mallion



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Docking Studies of Porphyrin-based Photosensitizers on Rhombellanes

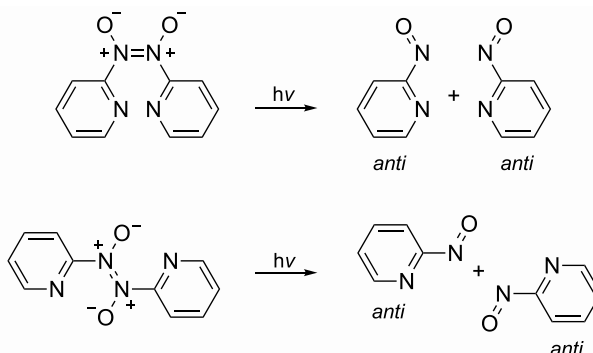
Raluca Pop, Mihai Medeleanu



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DOI: 10.5562/cca3789

Experimental and Theoretical IR Spectra of 2-Nitrosopyridines

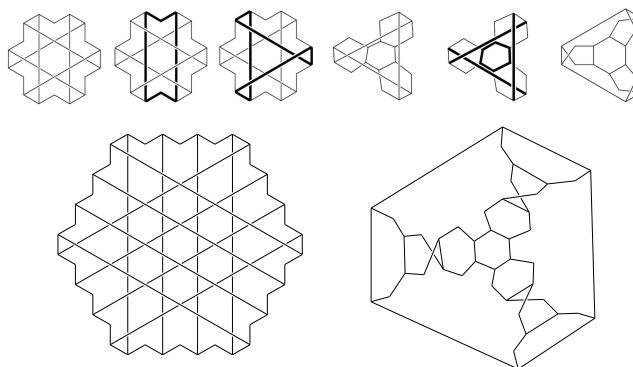
Katarina Varga, Hrvoj Vančik, Zlatko Mihalić



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DOI: 10.5562/cca3820

“Pure-Polyhex” π -Networks: Topo-Combinatorics

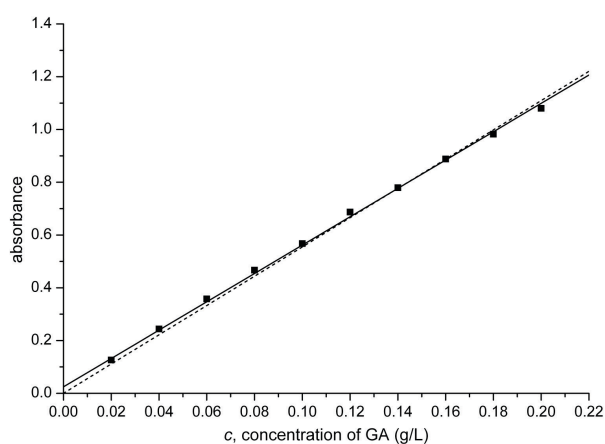
Douglas J. Klein, Bholanath Mandal

*Croat. Chem. Acta* **2020**, 93(4), 349–365

DOI: 10.5562/cca3790

Variations of Total Phenolic Content in Honey Samples Caused by Different Calibration Lines

Drago Bešlo, Klara Bešlo, Dejan Agić, Dražen Vikić-Topić, Bono Lučić

*Croat. Chem. Acta* **2020**, 93(4), 367–375

DOI: 10.5562/cca3805

OTHER PAPERS**In Memoriam: Mircea V. Diudea (1950 – 2019)**

Mihai V. Putz

Croat. Chem. Acta **2020**, 93(4), 377–378