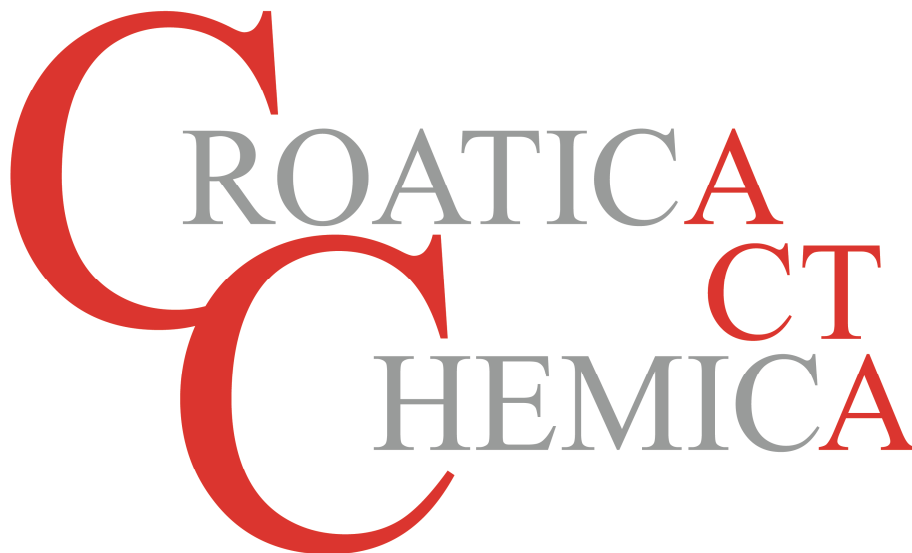


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Special Issue

The Klein Festschrift

On the occasion of 70th birthday of Professor Douglas Jay Klein

Guest Editors

Darko Babić Alexandru Teodor Balaban Bono Lučić Nenad Trinajstić

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*Festschrift in honour of
Professor Douglas Jay Klein
on the occasion of his 70th birthday*



Douglas Jay Klein

Professor at the Texas A&M University at Galveston

EDITORIAL

Darko Babić
Alexandru Teodor Balaban
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Croat. Chem. Acta **86** (2013) CCCCVII.

DOUGLAS JAY KLEIN – *Curriculum Vitae*

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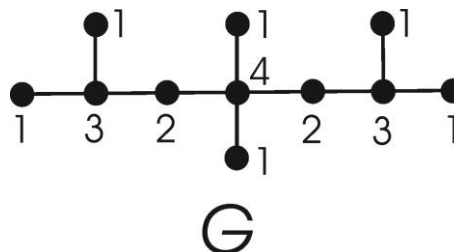
DOUGLAS JAY KLEIN – *List of Publications*

Croat. Chem. Acta **86** (2013)) CCCCXXI–CCCCXXXII.

FEATURE ARTICLE

Degree-Based Topological Indices

Ivan Gutman



Croat. Chem. Acta **86** (2013) 351–361.

ORIGINAL SCIENTIFIC ARTICLES

New Upper and Lower Bounds for the Additive Degree-Kirchhoff Index

Monica Bianchi, Alessandra Cornaro, José Luis Palacios,* and Anna Torriero

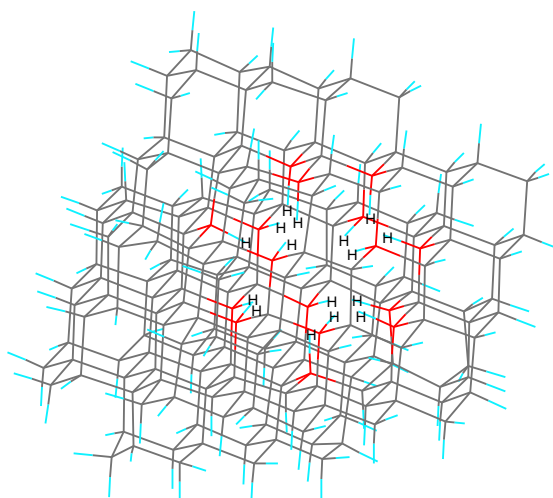
$$R^+(G) \geq N(N-4) + 2|E| \sum_{j=1}^N \frac{1}{d_j}$$

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Theoretical Study of Hole-Containing Macromolecular *Diamond Lattices* and Corona-*Diamondoid Molecules* or their Heteroatomic Derivatives

Alexandru T. Balaban

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Correlations of the Number of Dewar Resonance Structures and Matching Polynomials for the Linear and Zigzag Polyacene Series

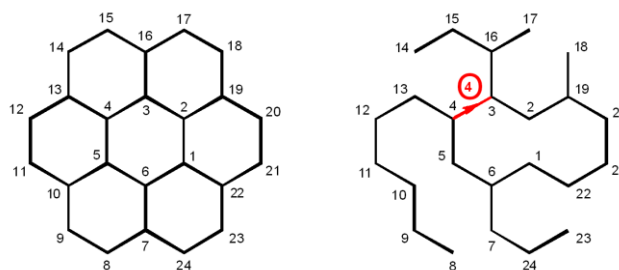
Jerry Ray Dias



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An Analysis of Topological Ring-Currents and their Use in Assessing the Annulene-Within-an-Annulene Model for Super-Ring Conjugated Systems

T. K. Dickens and R. B. Mallion*

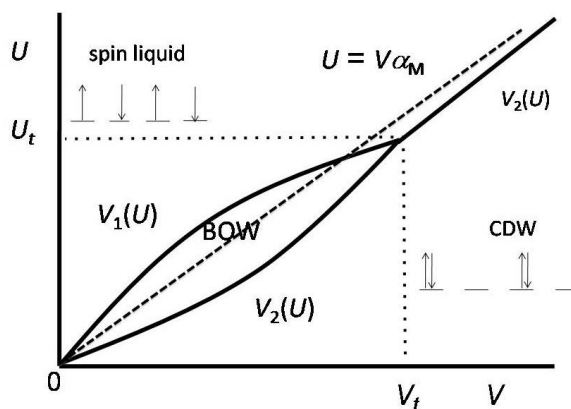


Croat. Chem. Acta **86** (2013) 387–406.

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Quantum Phase Diagram of One-Dimensional Spin and Hubbard Models with Transitions to Bond Order Wave Phases

Manoranjan Kumar, S. Ramasesha, and Zoltán G. Soos*



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From the Hubbard to the PPP Model

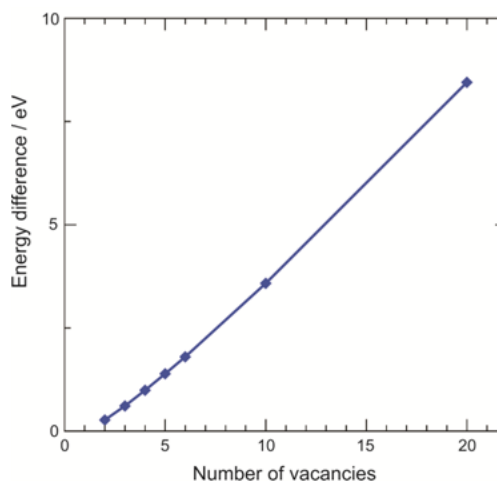
Thomas G. Schmalz

$$H^{\text{Hub}} = \sum_i t_{ii} E_{ii} + \sum_{ij} t_{ij} E_{ij} + \sum_i U_i n_{i\alpha} n_{i\beta} + \frac{1}{2} \sum_{ij} V_{ij} (Z_i - n_i)(Z_j - n_j) + V_c$$

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Model for the Formation of Helium Bubbles in Palladium

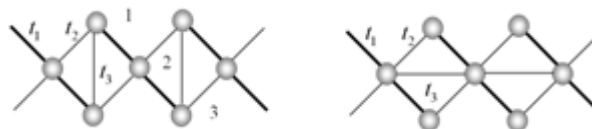
Julio Alfonso Alonso* and Andrés Ayuela



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$U = \infty$ Hubbard Model for 1D Frustrated Magnets

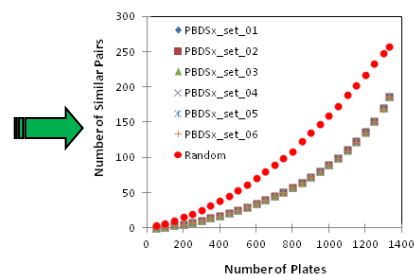
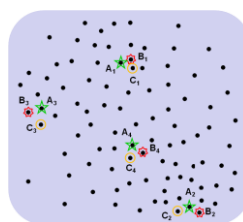
Vladyslav Olegovich Cheranovskii* and Elena Vladymirovna Ezerskaya



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A Heuristic Algorithm for Plate Selection That Maximizes Compound Diversity

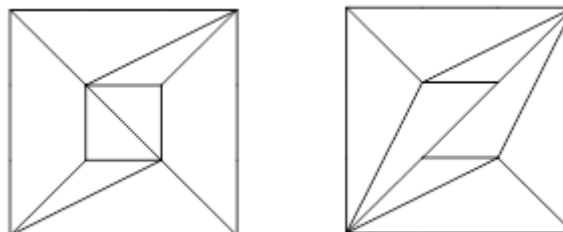
Hongyao Zhu,* Jacquelyn Klug-McLeod, and Gregory A. Bakken



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Distance Polynomial and the Related Counting Polynomials

Haruo Hosoya

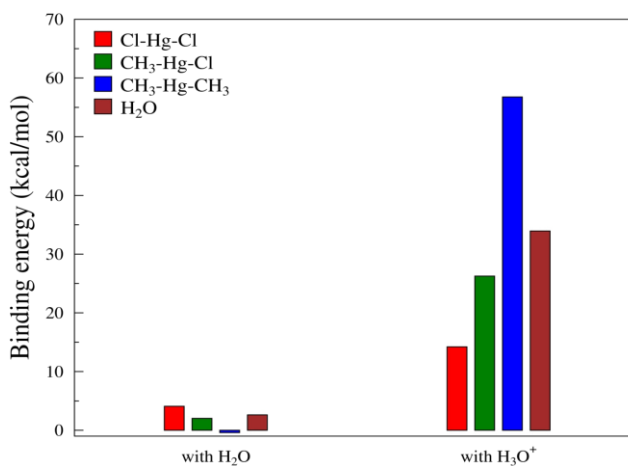


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Stability of Dimethylmercury and Related Mercury-containing Compounds with Respect to Selected Chemical Species Found in Aqueous Environment

Laimutis Bytautas

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Néel Temperature of Antiferromagnets for Phase Transitions Driven by Spin-wave Interactions

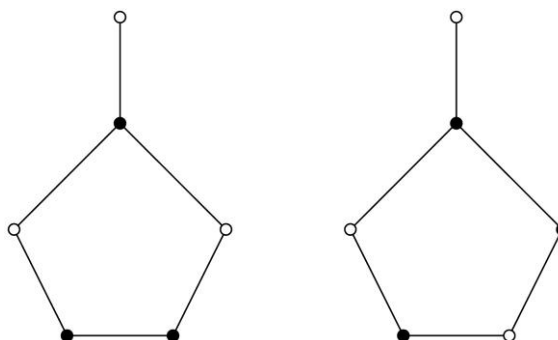
Andrés Ayuela,* Douglas J. Klein, and Norman H. March

$$\frac{\partial \langle n \rangle}{\partial \mu} = \langle n^2 \rangle \kappa_T = \beta S_{nn} \quad \chi_{ij} = \frac{\partial \langle m_i \rangle}{\partial h_j} = \lim_{q \rightarrow 0} \beta G_{ij}(q)$$

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Forcing Independence

Craig Larson* and Nico Van Cleemput

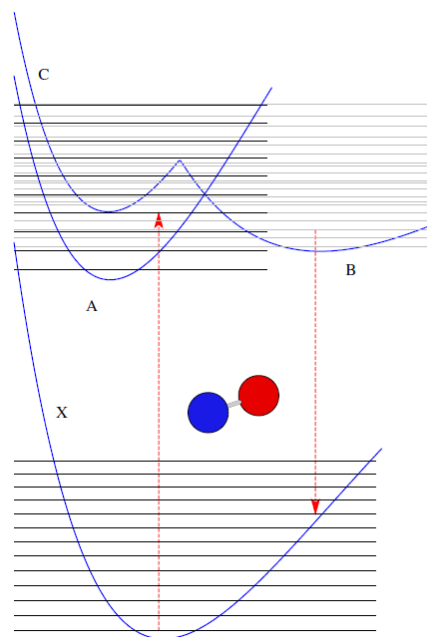


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Low-lying Adiabatic Electronic States of NO: a QMC Study

Luigi Giannellia and Claudio Amovilli

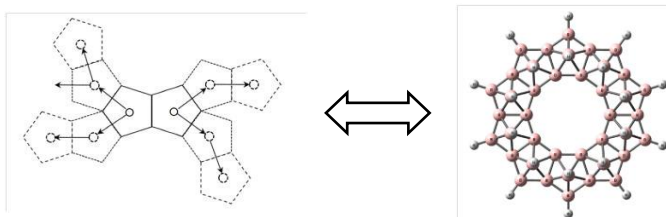
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Borane Polyhedra as Building Blocks for Unknown but Potentially Isolatable New Molecules – Extensions based on Computations of the Known B₁₈H₂₂ Isomers

Josep M. Oliva,* Juanjo Rué, Drahomír Hnyk, John D. Kennedy, and Vladimir R. Rosenfeld

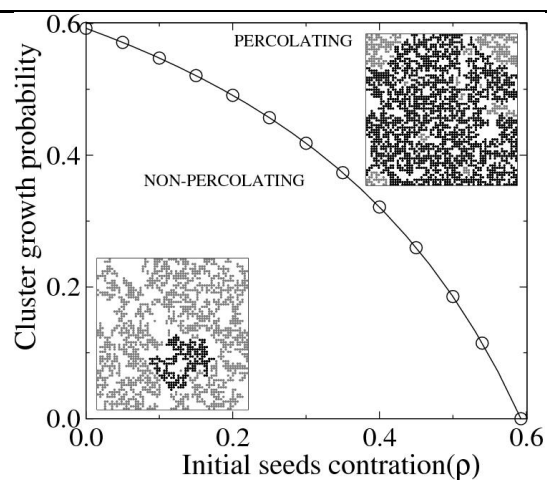
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Continuous Percolation Transition in Random Cluster Growth Model

Bappaditya Roy and Sitangshu Bikas Santra*

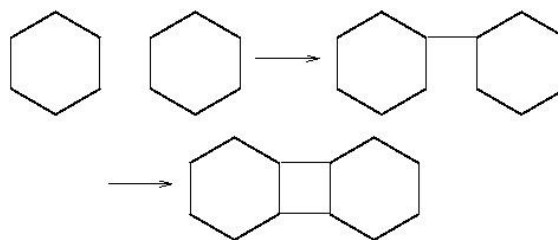
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On the Narumi-Katayama Index of Composite Graphs

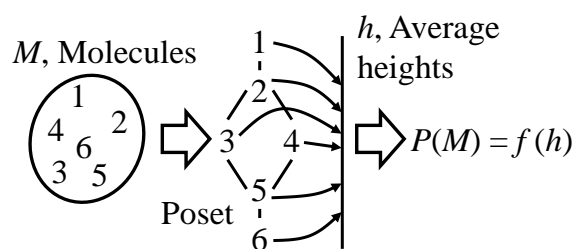
Mohammad Ali Hosseinzadeh, Ali Iranmanesh,*
and Tomislav Došlić



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Estimating Octanol / Water Partition Coefficients by Order Preserving Mappings

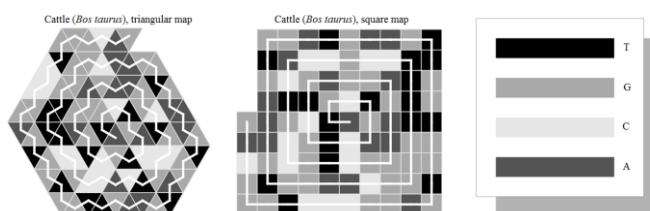
Rainer Bruggemann* and Guillermo Restrepo



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On Map Representations of DNA

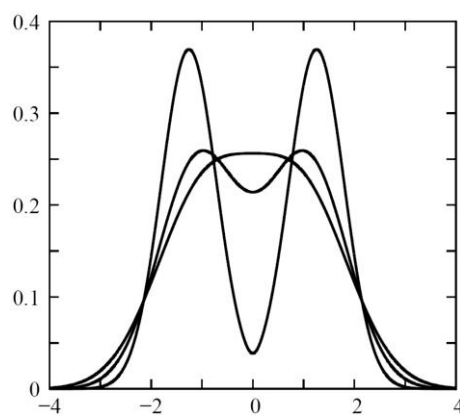
Milan Randić,* Boris Horvat, Gašper Jaklič, Dejan
Plavšić, and Tomaž Pisanski



Croat. Chem. Acta **86** (2013) 519–529.

Some Remarks on the Mass Density Distribution

Jacek Karwowski

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NOTES AND ESSAY

Reduced Matrix Elements for Symmetry-Constructed Systems

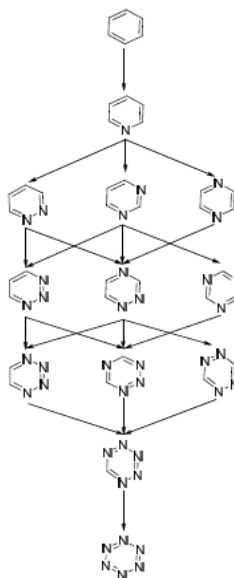
Marion Lawrence Ellzey, Jr

$$[H_0] = \begin{bmatrix} \alpha/2 & \beta & 0 \\ \beta & \alpha/2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

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A Note on the Substitution Reaction Network of Azines

Anirban Panda

Croat. Chem. Acta **86** (2013) 545–553.*Croat. Chem. Acta* **86** (2013) CCCCXVII.

Color Symmetry, Semigroups, Fractals

Vladimir R. Rosenfeld

Croat. Chem. Acta **86** (2013) 555–559.

APPENDICES

Personal Note

Guillermo Restrepo

CCCCXXXIII

Conclusion

CCCCXXXV