

DOUGLAS JAY KLEIN – *Curriculum Vitae*

Professor Douglas Jay Klein was born on November 8, 1942 in Portland, Oregon. He got his B.Sc. degree in Chemistry at the Oregon State University, Corvallis in 1964. His postgraduate studies were completed at the University of Texas at Austin, where he got M.A. degree in Physical Chemistry in 1967 and Ph.D. in 1969. After obtaining the Ph.D. degree, he spent the next ten years at the University of Texas in Austin, the University of Cologne, Princeton University, and Rice University in Houston. In 1979, he joined Texas A&M University at Galveston (TAMUG) as an Assistant Professor, soon to be promoted to a position of Associate Professor and in 1987 he became Full Professor.

Professor Klein's research covers very diverse topics. Topics of his research interest are many, e.g., electronic structure of organic polymers, electron correlation in models for organic molecules, many-body valence-bond theory, chemical graph theory, theory of elemental carbon clusters, partial orderings in chemistry, theory of defects in extended structures, polymer statistics and excluded volume, group-theoretic methods in chemistry and physics, fractal structures in the natural sciences, anomalous diffusion, population dynamics models.

His research is supported by grants from the Welch Foundation in Houston. He has been an active member of the following societies: American Chemical Society, American Physical Society, Mathematical Association of America, American Mathematical Society and International Society for Mathematical Chemistry. Professor Klein is also Fellow of the International Academy of Mathematical Chemistry.

He was engaged as a referee for a number of journals, e.g. *Croatica Chemica Acta*, *Journal of Mathematical Chemistry*, *International Journal of Quantum Chemistry*, *Journal of Chemical Information and Computer Science*, *MATCH Communications in*

Mathematical and in Computer Chemistry, *Physical Review B*, *Journal of the American Chemical Society*, *Theoretica Chimica Acta*, *Journal of the Chemical Society*, *Journal of Physics A*, *Journal of Chemical Education*, *Physical Review Letters*, *Discrete Applied Mathematics*, *Chemical Physics Letters*, *Journal of Chemical Physics*. He was also reviewer for some granting agencies, including NSF.

Professor Klein also edited two books: D. J. Klein and N. Trinajstić, *Valence-Bond Theory and Chemical Structure* (Elsevier, Amsterdam, 1990) and D. J. Klein and M. Randić, *Mathematical Chemistry* (VCH Pub., New York, 1990).

He also edited special issues of the following journals: D. J. Klein and M. Randić, *Journal of Mathematical Chemistry* 7 (1990) dedicated to the 3rd International conference on Mathematical Chemistry, D. J. Klein and J. Brickmann, special issue of *MATCH Communications in Mathematical Chemistry and in Computer Chemistry* vol. 42 (2000) dedicated to applications of partial orderings in chemistry and D. J. Klein, special issue of *Internet Electronic Journal of Molecular Design*, vol. 11 (2003) dedicated to Professor Nenad Trinajstić.

He was given the TAMU distinguished achievements award in research (1992), and Fulbright Fellowship at Oxford (1994).

Professor Klein was a member of the following Editorial Advisory Boards: *Journal of Mathematical Chemistry* (1988–2006), *MATCH Communications in Mathematical and in Computer Chemistry* (1994–), *International Journal of Quantum Chemistry* (1990–1993), *Fullerene Science & Technology* (1994–2003) and *Croatica Chemica Acta* (1995–).

Nenad Trinajstić

DOUGLAS JAY KLEIN – *List of Publications*

Scientific Articles

1. D. J. Klein, E. M. Greenawalt & F. A. Matsen, "The adjustment of Ab Initio Potential Curves", *Journal of Chemical Physics* **47** (1967) 4820–4823.
2. D. J. Klein, C. E. Rodriguez, J. C. Browne & F. A. Matsen, "The Ground-State of He²", *Journal of Chemical Physics* **47** (1967) 4862–4863.
3. F. A. Matsen & D. J. Klein, "Spin-Free Quantum Chemistry. VI. Spin Conservation", *Journal of Physical Chemistry* **73** (1969) 2477–2487.
4. D. J. Klein, "Local Permutational Symmetry and the Separated Atom Limit", *Journal of Chemical Physics* **50** (1969) 5140–5150.
5. D. J. Klein, "The Interaction of Two Metastable Triplet Helium Atoms", *Journal of Chemical Physics* **50** (1969) 5151–5157.
6. F. A. Matsen & D. J. Klein, "Spin Conservation", pages 1–55 in *Advances in Photochemistry*, Vol. VII, ed. by W. A. Noyes, Jr., G. S. Hammond and J. N. Pitts, Jr., (John Wiley and Sons, 1969).
7. D. J. Klein & R. W. Kramling, "The Symmetry of Reduced Density Matrices. I. General Algebraic Formulation", *International Journal of Quantum Chemistry S* **4** (1970) 661–674.
8. D. J. Klein, "The Symmetry of Reduced Density Matrices. II. Spin-Free Quantum Chemistry and Point Group Symmetry", *International Journal of Quantum Chemistry S* **3** (1970) 675–688.
9. D. J. Klein, C. H. Carlisle & F. A. Matsen, "Symmetry Adaptation to Sequences of Finite Groups", pages 219–260 in *Advances in Quantum Chemistry*, Vol. 5, ed. P. O. Lowdin (Academic Press, 1970).
10. D. J. Klein, "Symmetry Adapted Perturbation Theory for Interatomic and Intermolecular Exchange Energies", *International Journal of Quantum Chemistry S* **4** (1971) 271–283.
11. D. J. Klein, R. D. Poshusta, B. R. Junker & F. A. Matsen, "Computation in the Spin-Free Formulation of the Polyelectronic Problem", *International Journal of Quantum Chemistry S* **4** (1971) 141–146.
12. D. J. Klein & B. R. Junker, "Spin-Free Computation of Matrix Elements I: Group Theoretical Computation of Pauling Numbers", *Journal of Chemical Physics* **54** (1971) 4290–4296.
13. D. J. Klein & Z. G. Soos, "Site Representation for Charge Transfer Excitations in Molecular Crystals", *Molecular Physics* **20** (1971) 1013–1024.
14. D. J. Klein, "Variational Scheme for Multistate Kets", *Physical Review A* **3** (1971) 528–532.
15. F. A. Matsen & D. J. Klein, "Spin-Free Quantum Chemistry. IX. The Aggregate Theory of Polyelectronic Systems", *Journal of Physical Chemistry* **75** (1971) 1860–1865.
16. F. A. Matsen, D. J. Klein & D. C. Foyt, "Spin-Free Quantum Chemistry. X. The effective Spin Hamiltonian", *Journal of Physical Chemistry* **75** (1971) 1866–1873.
17. Z. G. Soos & D. J. Klein, "Modified Hubbard Model for Complex TCNQ Salts", *Journal of Chemical Physics* **55** (1971) 3284–3290.
18. B. R. Junker & D. J. Klein, "Spin-Free Computation of Matrix Elements II: Simplifications Due to Invariance Groups", *Journal of Chemical Physics* **55** (1971) 5532–5542.
19. D. J. Klein, D. Hankins, and R. W. Kramling, "Simple Construction of Point Group Degenerate Wave Functions", *International Journal of Quantum Chemistry* **6** (1972) 1101–1117.
20. W. A. Seitz & D. J. Klein, "Computations on Heisenberg Spin Models", *International Journal of Quantum Chemistry* **7** (1973) 647–665.
21. D. J. Klein, "A Group-Theoretic View of Weakly Interacting Sites", pages 193–207 in *Wave Mechanics – The First Fifty Years*, ed. W. C. Price, S. S. Chissick and T. Ravendale (Butterworth and Co., London, 1973).
22. D. J. Klein & W. A. Seitz, "Perturbation Expansion of the Linear Hubbard Model", *Physical Review B* **8** (1973) 2236–2247.
23. D. C. Foyt & D. J. Klein, "Multistate Kets for the Hydrogen Molecule", *Physical Review A* **8** (1973) 2274–2279.
24. D. J. Klein & D. C. Foyt, "Variational Multistate Ket Derivation of the Heisenberg Spin Hamiltonian", *Physical Review A* **8** (1973) 2280–2287.
25. D. J. Klein, "Degenerate Perturbation Theory", *Journal of Chemical Physics* **61** (1974) 786–798.
26. D. J. Klein, "Atomic Limit and Projected Hubbard Models for Linear Chain", *Physical Review B* **8** (1973) 3452–3458.
27. D. J. Klein & A. A. Cantu, "Symmetry Adaptation and the Relation between the Spin-Free and Space-Spin Formulations of Electronic Structure", *International Journal of Quantum Chemistry* **8** (1974) 223–233.
28. D. J. Klein, "Comments on Kets not Strongly Symmetry Adapted", *International Journal of Quantum Chemistry* **8** (1974) 234–245.
29. W. A. Seitz & D. J. Klein, "Static Thermodynamic Properties of the Linear Half-filled Hubbard Model", *Physical Review B* **9** (1974) 2159–2164.
30. D. J. Klein, "Finite Groups and Semisimple Algebras in Quantum Mechanics", pages 1–93 in *Group Theory and Its Applications*, Vol. III, ed. E. M. Loebl (Academic Press, New York, 1975).
31. D. J. Klein & W. A. Seitz, "Partially Filled Linear Hubbard Model Near the Atomic Limit", *Physical Review B* **10** (1974) 3217–3226.

32. D. J. Klein, "Kets of Broken Symmetry in the Derivation of Model Hamiltonians", *Revista Mexicana Fisica* **23** (1974) 243–256.
33. D. J. Klein & A. H. Cowley, "Permutational Isomerism", *Journal of the American Chemical Society* **97** (1975) 1633–1640.
34. Z. G. Soos & D. J. Klein, "Charge-Transfer in Solid State Complexes", pages 1–109 in *Molecular Associations*, Vol. I, (Academic Press, New York, 1975).
35. A. A. Cantu, D. J. Klein, F. A. Matsen & T. H. Seligman, "A Second-Quantized Formulation of Valence-Bond Theory", *Theoretica Chimica Acta* **38** (1975) 341–354.
36. G. Ananthkrishna, L. F. Weiss, D. C. Foyt & D. J. Klein, "Properties of the Linear Heisenberg Chain with Nearest and Next-Nearest Neighbor Interactions", *Physica B* **81** (1976) 275–284.
37. D. J. Klein, "Variational Localized-Site Cluster Expansions. I. General Theory", *Journal of Chemical Physics* **64** (1976) 4868–4872.
38. D. J. Klein & M. A. Garcia-Bach, "Variational Localized-Site Cluster Expansions. II. Trees and Near-Trees", *Journal of Chemical Physics* **64** (1976) 4873–4877.
39. D. J. Klein, "Variational Localized-Site Cluster Expansions. III. Point Group Symmetry and Supersymmetry", *Molecular Physics* **31** (1976) 783–796.
40. D. J. Klein & M. A. Garcia-Bach, "Variational Localized-Site Cluster Expansions. IV. Hubbard and PPP Models", *Molecular Physics* **31** (1976) 797–809.
41. D. J. Klein, "Variational Localized-Site Cluster Expansion. V. Valence-Bond and Heisenberg Models", *Molecular Physics* **31** (1976) 811–823.
42. D. J. Klein & H. M. Pickett, "Nodal Hypersurfaces and Anderson's Random-Walk Simulation of the Schroedinger Equation", *Journal of Chemical Physics* **64** (1976) 4811–4812.
43. Z. G. Soos & D. J. Klein, "Organic Molecular Crystals: Charge Transfer Complexes", pages 679–788 in *Treatise on Solid State Chemistry*, Vol. 3 ed. N. B. Hannay (Plenum Press, New York, 1976).
44. W. Hasselbarth, E. Ruch, D. J. Klein & T. H. Seligman, "Double Classes: A New Classification Scheme for Group Elements", pages 617–622 in *Proceedings of the V International Colloquium on Group Theory and Its Applications*, ed. R. T. Sharpe (Academic Press, New York, 1977).
45. D. J. Klein, "Variational Localized-Site Cluster Expansions. VI. General Theory Revisited", *International Journal of Quantum Chemistry* **11** (1977) 255–271.
46. M. A. Garcia-Bach & D. J. Klein, "Variational Localized-Site Cluster Expansions. VII. Higher Ansatzes and the Linear Heisenberg Model", *International Journal of Quantum Chemistry* **11** (1977) 273–289.
47. D. J. Klein & M. A. Garcia-Bach, "Variational Localized-Site Cluster Expansions. VIII. Projection of Spin Symmetries", *International Journal of Quantum Chemistry* **11** (1977) 291–303.
48. D. J. Klein & P. L. DeVries, "Satisfying Certain Matrix Element Formulas", *Journal of Chemical Physics* **68** (1978) 160–162.
49. D. J. Klein & A. H. Cowley, "Permutational Isomerism with Bidentate Ligands and Other Constraints", *Journal of the American Chemical Society* **100** (1978) 2593–2599.
50. D. J. Klein, "Variational Localized-Site Cluster Expansions. IX. Many-Body Valence-Bond Theory", *Physical Review B* **19** (1979) 870–876.
51. D. J. Klein & M. A. Garcia-Bach, "Variational Localized-Site Cluster Expansions. X. Dimerization in Linear Chains", *Physical Review B* **19** (1979) 877–886.
52. F. T. Wall & D. J. Klein, "Comment on Self-Avoiding Walks on Strips", *Proceedings of the National Academy of Sciences, U.S.A.* **76** (1979) 1529–1531.
53. D. J. Klein, "Long-Range-Order of Spin-Pairing in Valence-Bond Theory", *International Journal of Quantum Chemistry S* **13** (1979) 293–303.
54. W. Hasselbarth, E. Ruch, D. J. Klein & T. H. Seligman, "Bilateral Classes", *Journal of Mathematical Physics* **21** (1980) 951–953.
55. D. J. Klein, "Distributions for Self-Avoiding Walks on Strips, Cylinders, and Tubes", *Journal of Statistical Physics* **23** (1980) 561–586.
56. D. J. Klein & T. L. Welscher, "Cluster Expansion and Generalized Transfer Matrices for the Statistical Mechanics of Linear Chains", *Journal of Statistical Physics* **24** (1981) 555–586.
57. D. J. Klein, "Extension of the Dirac Identity", *Journal of Physics A* **13**(1980) 3141–3146.
58. D. J. Klein, "Rigorous Results for a Branched Polymer Model Including Volume Exclusion", *Journal of Chemical Physics* **75** (1981) 5186–5189.
59. W. A. Seitz & D. J. Klein, "Monte Carlo Results for a Branched Polymer Model Including Volume Exclusion", *Journal of Chemical Physics* **77** (1981) 5190–5193.
60. D. J. Klein, "Ground-State Features of Heisenberg Models", *Journal of Chemical Physics* **77** (1982) 3098–3100.
61. D. J. Klein, C. Nelin, S. Alexander & F. A. Matsen, "High-Spin Hydrocarbons", *Journal of Chemical Physics* **77** (1982) 3101–3108.
62. D. J. Klein, "Treediagonal Matrices and Their Inverses", *Linear Algebra and Its Applications* **42** (1982) 109–117.
63. M. A. Garcia-Bach & D. J. Klein, "Ground-State of the Antiferromagnetic Heisenberg Chain with Nearest- and Next-Nearest-Neighbors Interactions", *Physics Letters A* **89** (1982) 101–102.
64. R. D. Poshusta & D. J. Klein, "Novel Ab Initio Correlated Calculations for the Infinite Chain of Hydrogen Atoms", *Physical Review Letters* **48** (1982) 1555–1558.
65. D. J. Klein, "Exact Ground States for a Class of Antiferromagnetic Heisenberg Models with Short-range Interactions", *Journal of Physics A* **15** (1982) 661–671.
66. D. J. Klein, W. A. Seitz & J. E. Kilpatrick, "Branched Polymer Models", *Journal of Applied Physics* **53** (1982) 6599–6603.
67. D. J. Klein, "Valence-Bond Theory for Conjugated Hydrocarbons", *Pure & Applied Chemistry* **55** (1982) 299–306.
68. D. J. Klein & T. H. Seligman, "Wigner-Eckart Theorem for Induced Symmetries", *Kinam* **4** (1982) 349–378.
69. D. J. Klein & W. A. Seitz, "Self-similar Self-avoiding Structures Models for Polymers", *Proceedings of the National Academy of Science, U.S.A.* **80** (1983) 3125–3128.
70. E. Ruch & D. J. Klein, "Double Cosets in Chemistry and Physics", *Theoretica Chimica Acta* **63** (1983) 447–472.
71. D. J. Klein, W. A. Seitz, M. A. Garcia-Bach, J. M. Picone & D. C. Foyt, "Variational Localized-Site Cluster Expansions. XI. Coherent State Derivation of Effective Heisenberg Hamiltonians", *International Journal of Quantum Chemistry S* **17** (1983) 555–571.
72. D. J. Klein & W. A. Seitz, "Graphs, Polymer Models, Excluded Volume, and Chemical Reality", pages 430–445 in *Chemical Applications of Topology and Graph Theory*, ed. R. B. King (Elsevier, Amsterdam, 1983).
73. T. G. Schmalz, G. E. Hite & D. J. Klein, "Compact Self-avoiding

- Circuits on Two-Dimensional Lattices", *Journal of Physics A* **17** (1984) 445–453.
74. D. J. Klein, G. E. Hite, T. G. Schmalz & W. A. Seitz, "Spiralling Self-avoiding Walks", *Journal of Physics A* **17** (1984) L209–L214.
75. D. J. Klein, "Semiregular Induction of Group Representations", *Journal of Mathematical Physics* **25** (1984) 200–203.
76. D. J. Klein & W. A. Seitz, "Self-interacting Self-avoiding Walks on the Sierpinski Gasket", *Journal de Physique Lettres* **45** (1984) L241–L247.
77. D. J. Klein & N. Trinajstić, "Hückel Rules and Electron Correlation", *Journal of the American Chemical Society* **106** (1984) 8050–8056.
78. S. A. Alexander & D. J. Klein, "Ground-State Spin Pairing of General-Spin Linear-Chain Heisenberg Models", *Physical Review B* **31** (1985) 574–576.
79. W. A. Seitz, D. J. Klein, T. G. Schmalz & M. A. Garcia-Bach, "The Poly-Polyacene Family of Multi-Phase Pi-Network Polymers in a Valence-Bond Picture", *Chemical Physics Letters* **115** (1985) 139–143.
80. D. J. Klein, T. G. Schmalz, G. E. Hite, A. Metropoulos & W. A. Seitz, "The Poly-Polyphenanthrene Family of Multi-Phase Pi-Network Polymers in a Valence-Bond Picture", *Chemical Physics Letters* **120** (1985) 367–371.
81. D. J. Klein, T. G. Schmalz, W. A. Seitz & G. E. Hite, "Overview of Hückel and Resonance-Theoretic Approaches to Pi-Network Polymers", *International Journal of Quantum Chemistry S* **19** (1986) 707–718.
82. D. J. Klein, G. E. Hite & T. G. Schmalz, "Transfer-Matrix Method for Subgraph Enumeration: Application to Polypyrene Fusenes", *Journal of Computational Chemistry* **7** (1986) 443–456.
83. M. Randić, D. O. Oakland & D. J. Klein, "Symmetry Properties of Chemical Graphs. IX. The Valence-Tautomerism in the P73-Skeleton", *Journal of Computational Chemistry* **7** (1986) 35–54.
84. D. J. Klein, "Chemical Graph-Theoretic Cluster Expansions", pages 171–180 in *Mathematical and Computational Concepts in Chemistry*, ed. N. Trinajstić (Ellis-Horwood Pub., Chichester, England, 1986).
85. D. J. Klein, T. G. Schmalz, G. E. Hite & W. A. Seitz, "Resonance in C60 Buckminsterfullerene", *Journal of the American Chemical Society* **108** (1986) 1301–1302.
86. G. E. Hite, A. Metropoulos, D. J. Klein, T. G. Schmalz & W. A. Seitz, "Extended Pi-Networks with Multiple Spin-Pairing Phases: Resonance-Theory Calculations on Poly-polyphenanthrenes", *Theoretica Chimica Acta* **69** (1986) 369–392.
87. D. J. Klein, S. A. Alexander, W. A. Seitz, T. G. Schmalz & G. E. Hite, "Wavefunction Comparisons for the Valence-Bond Model for Conjugated Pi-Networks", *Theoretica Chimica Acta* **69** (1986) 393–408.
88. D. J. Klein, G. E. Hite, W. A. Seitz & T. G. Schmalz, "Dimer Coverings and Kekulé Structures on Honeycomb Lattice Strips", *Theoretica Chimica Acta* **69** (1986) 409–420.
89. T. G. Schmalz, W. A. Seitz, D. J. Klein & G. E. Hite, "C60 Carbon Cages", *Chemical Physics Letters* **130** (1986) 203–207.
90. M. Randić & D. J. Klein, "Kekulé Valence Structures Revisited. Innate Degrees of Freedom of Pi-Electron Couplings", pages 274–282 in *Mathematical and Computational Concepts in Chemistry*, ed. N. Trinajstić (Ellis-Horwood Pub., Chichester, England, 1986).
91. D. J. Klein, W. A. Seitz & T. G. Schmalz, "Icosahedral-Symmetry Carbon Cages", *Nature* **323** (1986) 703–706.
92. N. Trinajstić, M. Randić & D. J. Klein, "On the Quantitative Structure-Activity Relationship in Drug Research", *Acta Pharmaceutica Jugoslavica* **36** (1986) 267–279.
93. D. J. Klein, "Chemical Graph-Theoretic Cluster Expansions", *International Journal of Quantum Chemistry S* **20** (1986) 153–171.
94. N. Trinajstić, D. J. Klein & M. Randić, "On Some Solved and Unsolved Problems of Chemical Graph Theory", *International Journal of Quantum Chemistry S* **20** (1986) 699–742.
95. D. J. Klein & M. Randić, "Innate Degree of Freedom of a Graph", *Journal of Computational Chemistry* **8** (1987) 516–521.
96. D. J. Klein & S. A. Alexander, "Organic Polyradicals, High-Spin Hydrocarbons, and Organic Ferromagnets", pages 404–419 in *Chemical Applications of Topology and Graph Theory*, ed. R. B. King (Elsevier Pub., Amsterdam, 1987).
97. M. Randić, V. Solomon, S. C. Grossman, D. J. Klein & N. Trinajstić, "Resonance Energies of Large Conjugated Hydrocarbons by a Statistical Method", *International Journal of Quantum Chemistry* **32** (1987) 35–59.
98. W. A. Seitz, G. E. Hite, T. G. Schmalz & D. J. Klein, "Resonance in Poly-polyphenanthrenes: A Transfer Matrix Approach", pages 458–465 in *Chemical Applications of Graph Theory and Topology*, ed. R. B. King & D. H. Rouvray (Elsevier, Amsterdam, 1987).
99. M. Randić, D. J. Klein, V. Katović, D. O. Oakland, W. A. Seitz & A. T. Balaban, "Symmetry Properties of Chemical Graphs. X. Rearrangement of Axially Distorted Octahedra", pages 266–284 in *Chemical Applications of Graph Theory and Topology*, Ed. R. B. King and D. H. Rouvray (Elsevier, Amsterdam, 1987).
100. D. J. Klein, T. P. Živković & N. Trinajstić, "Resonance in Random Pi-Network Polymers", *Journal of Mathematical Chemistry* **1** (1987) 309–334.
101. D. J. Klein, "Exchange Perturbation Theories", *International Journal of Quantum Chemistry* **32** (1987) 337–396.
102. W. A. Seitz, D. J. Klein & T. G. Schmalz, "Elemental Carbon Cages" in *Proceedings of the 18th Biennial Conference on Carbon* (Worcester Polytechnic Institute Press, Worcester, Massachusetts, 1987).
103. T. G. Schmalz, W. A. Seitz, D. J. Klein & G. E. Hite, "Elemental Carbon Cages", *Journal of the American Chemical Society* **110** (1988) 1113–1127.
104. T. G. Schmalz, T. Živković & D. J. Klein, "Cluster Expansion of the Hückel Molecular Energy of Acyclics: Applications to Pi Resonance Theory" pages 173–190 in *MATH/CHEM/COMP 1987*, ed. R. C. Lacher (Elsevier Pub., Amsterdam, 1988).
105. W. A. Seitz, D. J. Klein & A. Graovac, "Transfer Matrix Methods for Regular Polymer Graphs" pages 157–171 in *MATH/CHEM/COMP 1987*, ed. R. C. Lacher (Elsevier Pub., Amsterdam, 1988).
106. D. J. Klein, W. C. Herndon & M. Randić, "On the Classification of Polyhex Polymers", *New Journal of Chemistry* **12** (1988) 71–76.
107. S. A. Alexander & D. J. Klein, "High-Spin Carbenes", *Journal of the American Chemical Society* **110** (1988) 3401–3405.
108. D. J. Klein & W. A. Seitz, "Pauling-Wheland Resonance Theory of Benzenoid Hydrocarbons", *Journal of Molecular Structure (Theochem)* **169** (1988) 167–181.
109. D. J. Klein, T. G. Schmalz, S. El-Basil, M. Randić & N. Trinajstić, "Kekulé Count and Algebraic Structure Count for Unbranched Alternate Catafusenes", *Journal of Molecular Structure (Theochem)* **179** (1988) 99–107.
110. G. E. Hite, T. P. Živković & D. J. Klein, "Conjugated Circuit Theory for Graphite", *Theoretica Chimica Acta* **74** (1988)

- 349–361.
111. W. A. Seitz, D. J. Klein & G. E. Hite, "Interacting dimers on a Sierpinski gasket", *Discrete Applied Mathematics* **19** (1988) 339–348.
 112. R. D. Poshusta, T. G. Schmalz & D. J. Klein, "Heisenberg-Model Cluster Expansion for Half-filled Hubbard and PPP Models", *Molecular Physics* **66** (1989) 317–332.
 113. D. J. Klein & T. G. Schmalz, "Exact Ground State for a Herndon-Simpson Model via Resonance-Theoretic Cluster Expansion", *International Journal of Quantum Chemistry* **35** (1989) 373–383.
 114. D. J. Klein & W. A. Seitz, "Transfer-Matrix Approximants: The Chromatic Polynomial", pages 155–166 in *MATH/CHEM/COMP 1988*, ed. A. Graovac (Elsevier, Amsterdam, 1988).
 115. D. J. Klein, M. A. Garcia-Bach & W. A. Seitz, "Variational Localized-Site Cluster Expansion 16. Excitations", *Journal of Molecular Structure (Theochem)* **185** (1989) 275–285.
 116. M. A. Garcia-Bach, R. Valenti & D. J. Klein, "Covalent Excitations of a Polyphene Polymer via a Herndon-Simpson Model", *Journal of Molecular Structure (Theochem)* **185** (1989) 287–296.
 117. S. El-Basil & D. J. Klein, "Fibonacci numbers in the Topological Theory of Benzenoid Hydrocarbons and Related Graphs", *Journal of Mathematical Chemistry* **3** (1989) 1–23.
 118. S. Nikolić, M. Randić, D. J. Klein, D. Plavšić & N. Trinajstić, "The Conjugated-Circuit Model: Application to Benzenoid Hydrocarbons", *Journal of Molecular Structure* **198** (1989) 223–237.
 119. D. J. Klein & N. Trinajstić, "Foundations of conjugated-circuits models", *Pure & Applied Chemistry* **61** (1989) 2107–2115.
 120. D. J. Klein, "Semiempirical Valence-Bond Views for Benzenoid Hydrocarbons", *Topics in Current Chemistry* **153** (1990) 57–83.
 121. N. Trinajstić, D. Plavšić & D. J. Klein, "The Conjugated-Circuit Model Revisited", *Croatica Chimica Acta* **62** (1989) 711–718.
 122. R. S. Chen, S. J. Cyvin, B. N. Cyvin, J. Brunvoll & D. J. Klein, "Methods of Enumerating Kekulé Structures, Exemplified by Application to Rectangle-Shaped Benzenoids", *Topics in Current Chemistry* **15** (1990) 227–253.
 123. D. J. Klein, S. A. Alexander & M. Randić, "Polyradicals and High-Spin Hydrocarbons", *Molecular Crystals & Liquid Crystals* **176** (1989) 109–114.
 124. D. J. Klein, M. A. Garcia-Bach & R. Valenti, "Neutral Excitations in Quasi-1-D Strongly Correlated Electron Systems", *International Journal of Modern Physics B* **3** (1989) 2159–2168.
 125. D. J. Klein & T. G. Schmalz, "Exact Enumeration of Long-Range-Ordered Dimer Coverings of the Square-Planar Lattice", *Physical Review B* **41** (1990) 2244–2248.
 126. T. P. Živković, B. J. Sandleback, T. G. Schmalz & D. J. Klein, "Heisenberg Model for the Square-Planar Lattice and Fragments", *Physical Review B* **41** (1990) 2249–2256.
 127. D. J. Klein & T. P. Živković, "Graphical and Color-Pairing Symmetries", *International Journal of Quantum Chemistry* **37** (1990) 423–436.
 128. D. J. Klein, W. A. Seitz & T. G. Schmalz, "Conjugated-Circuit Computations for Conjugated Hydrocarbons" pages 128–147 in *Computational Graph Theory*, Ed. D. H. Rouvray (Nova Science Publishers, New York, 1990).
 129. D. J. Klein & N. Trinajstić, "Pascal Recurrence Algorithm for Kekulé-Structure Counts of Benzenoid and Coronoid Hydrocarbons", *Journal of Molecular Structure (Theochem)* **206** (1990) 135–142.
 130. D. J. Klein & N. Trinajstić, "Valence-Bond Theory and Chemical Structure", *Journal of Chemical Education* **67** (1990) 633–637.
 131. D. J. Klein & T. G. Schmalz "Buckminsterfullerene, Part A: Introduction" pages 239–246 in *Quasicrystals, Networks, and Molecules of Fivefold Symmetry*, Edited by I. Hargittai (VCH Pub., New York, 1990).
 132. E. Brensdal, S. J. Cyvin, B. N. Cyvin, J. Brunvoll, D. J. Klein & W. A. Seitz "Buckminsterfullerene, Part C: Hückel Energy Levels", pages 257–264 in *Quasicrystals, Networks, and Molecules of Fivefold Symmetry*, Ed. I. Hargittai (VCH Pub., New York, 1990).
 133. V. Elser, E. Brensdal, S. J. Cyvin, J. Brunvoll, B. N. Cyvin & D. J. Klein, "Buckminsterfullerene, Part D: Kekulé Structures", pages 265–276 in *Quasicrystals, Networks, and Molecules of Fivefold Symmetry*, Ed. I. Hargittai (VCH Pub., New York, 1990).
 134. S. Nikolić, N. Trinajstić & D. J. Klein, "The Conjugated-Circuit Model", *Computers in Chemistry* **14** (1990) 313–322.
 135. D. J. Klein, "Hückel-Model Solution for Polyphenanthrene Strips", *Reports of Molecular Theory* **1** (1990) 91–94.
 136. R. D. Poshusta, D. J. Klein & J. Meikelburger, "Ground-State Real-Space Renormalization for Linear-Chain Heisenberg Models with Alternation", *Physica A* **170** (1991) 265–277.
 137. N. Trinajstić, T. G. Schmalz, T. P. Živković, S. Nikolić, G. E. Hite, D. J. Klein & W. A. Seitz, "[N]-Phenylenes: A Theoretical Study", *New Journal of Chemistry* **15** (1991) 27–31.
 138. D. J. Klein, T. P. Živković & R. Valenti, "Topological Long-range Order for Resonating Valence-Bond Structures", *Physical Review B* **43** (1991) 723–727.
 139. D. J. Klein, T. G. Schmalz, M. A. Garcia-Bach, R. Valenti & T. P. Živković, "Resonating Valence-Bond Theory for the Square-Planar Lattice", *Physical Review B* **43** (1991) 719–722.
 140. I. Gutman & D. J. Klein, "Generalization of Cyvin's Formula", *Journal of Mathematical Chemistry* **6** (1991) 41–50.
 141. F. Harary, D. J. Klein & T. P. Živković, "Graphical Properties of Polyhexes: Perfect Matching Vector and Forcing", *Journal of Mathematical Chemistry* **6** (1991) 295–306.
 142. N. Trinajstić, S. Nikolić & D. J. Klein, "Quantum-Mechanical and Computational Aspects of the Conjugated-Circuit Model", *Journal of Molecular Structure (Theochem)* **229** (1991) 63–89.
 143. D. J. Klein & W. A. Seitz, "Directed Self-Interacting Self-Avoiding Random Walks" pages 403–416 in *Nonlinear Topics in Ocean Physics*, ed. A. R. Osborne (North-Holland, Amsterdam, 1991).
 144. D. J. Klein, "Comment on Average Kekulé-Structure Counts for random Conjugated Polymers", *Journal of Mathematical Chemistry* **6** (1991) 385–388.
 145. R. D. Poshusta & D. J. Klein, "Ab Initio Valence-Bond Cluster-Expansion for an Alternating Infinite Chain of Hydrogen Atoms", *Journal of Molecular Structure (Theochem)* **229** (1991) 103–113.
 146. S. J. Cyvin, B. N. Cyvin, J. Brunvoll, H. Hosoya, F. Zhang, D. J. Klein, R. Chen & O. E. Polansky, "Kekulé-Structure Counts: General Formulations for Primitive Coronoid Hydrocarbons", *Monatshefte für Chemie* **122** (1991) 435–444.
 147. D. J. Klein, M. J. Cravey & G. E. Hite, "Fractal Benzenoids", *Polycyclic Aromatic Compounds* **2** (1991) 163–182.
 148. D. J. Klein & W. A. Seitz, "Symmetric-Group Algebraic Variational Solutions for Heisenberg Models at Finite Temperature", *International Journal of Quantum Chemistry* **41** (1992) 43–52.
 149. X. Liu & D. J. Klein, "The Graph Isomorphism Problem", *Journal of Computational Chemistry* **12** (1991) 1243–1251.

150. X. Liu, D. J. Klein, T. G. Schmalz & W. A. Seitz, "Generation of Carbon-Cage Polyhedra", *Journal of Computational Chemistry* **12** (1991) 1252–1259.
151. D. J. Klein & X. Liu, "Many-Body Conjugated-Circuit Computations", *Journal of Computational Chemistry* **12** (1991) 1260–1264.
152. X. Liu, D. J. Klein, W. A. Seitz & T. G. Schmalz, "Sixty-Atom Carbon Cages", *Journal of Computational Chemistry* **12** (1991) 1265–1269.
153. T. G. Schmalz, D. J. Klein & B. L. Sandleback, "Chemical Graph Theoretic Cluster Expansion and Diamagnetic Susceptibility", *Journal of Chemical Information and Computer Sciences* **32** (1992) 54–57.
154. X. Liu, T. G. Schmalz & D. J. Klein, "Favorable Structures for Higher Fullerenes", *Chemical Physics Letters* **188** (1992) 550–554.
155. M. A. Garcia-Bach, R. Valenti, S. A. Alexander & D. J. Klein, "Resonating Valence-Bond Theory for Polyenes and Polyacetylene", *Croatica Chemica Acta* **64** (1991) 415–427.
156. W. A. Seitz & D. J. Klein, "Random Spirals", pages 83–94 in *Spiral Symmetry*, ed. I. Hargittai and C. A. Pickover (World Scientific, Singapore, 1992).
157. M. A. Garcia-Bach, A. Penaranda & D. J. Klein, "Valence-bond Treatment of Distortions in Polyacene Polymers", *Physical Review B* **45** (1992) 10891–10901.
158. D. J. Klein, Z. Mihalić, D. Plavšić & N. Trinajstić, "Molecular Topological Index: A relation with the Wiener Index", *Journal of Chemical Information and Computer Sciences* **32** (1992) 304–305.
159. D. J. Klein & A. T. Balaban, "Generalized Hückel-Möbius Rule", *Journal of Molecular Structure (Theochem)* **259** (1992) 307–315.
160. D. J. Klein & X. Liu, "Theorems for Carbon Cages", *Journal of Mathematical Chemistry* **11** (1992) 199–205.
161. T. G. Schmalz, D. J. Klein & X. Liu, "Favorable Structures for Higher Fullerenes", *Materials Research Society Symposium Proceedings* **270** (1992) 129–134.
162. D. Plavšić, N. Trinajstić & D. J. Klein, "Clar Structures in Fractal Benzenoids", *Croatica Chemica Acta* **65** (1992) 279–284.
163. D. J. Klein, "Aromaticity via Kekulé Structures and Conjugated Circuits", *Journal of Chemical Education* **69** (1992) 691–694.
164. T. G. Schmalz & D. J. Klein, "Fullerene Structures" pages 83–101 in *Buckminsterfullerenes* ed. W. E. Billups & M. A. Ciufolini (VCH Pub., New York, 1992).
165. D. J. Klein, W. A. Seitz & T. G. Schmalz, "Symmetry of Infinite Tubular Polymers: Application to Buckytubes", *Journal of Physical Chemistry* **97** (1993) 1231–1236.
166. A. T. Balaban, X. Liu, S. J. Cyvin & D. J. Klein, "Benzenoids with Maximum Kekule Structure Counts for Given Numbers of Hexagons", *Journal of Chemical Information and Computer Sciences* **33** (1993) 429–436.
167. D. J. Klein & M. Randić, "Resistance Distance", *Journal of Mathematical Chemistry* **12** (1993) 81–95.
168. D. Babić, D. J. Klein & C. H. Sah, "Symmetry of Fullerenes", *Chemical Physics Letters* **211** (1993) 235–241.
169. D. J. Klein & S. A. Alexander, "Biradical Spin, Limited CI and Heteroatoms", *Molecular Crystals & Liquid Crystals* **232** (1993) 219–232.
170. D. J. Klein & T. P. Živković, "Subgraph Generating Functions in Chemistry-An Example for Perfect Matching on Honeycomb Lattices", *Mathematical Computational Modeling* **17** (1993) 113–123.
171. T. G. Schmalz & D. J. Klein, "Renormalization Group for the Linear-Chain Heisenberg Model", *Croatica Chemica Acta* **66** (1993) 185–192.
172. D. J. Klein, T. P. Živković & A. T. Balaban, "The Fractal Family of Coro[N]enes", *Communications in Mathematical Chemistry (MatCh)* **29** (1993) 107–130.
173. D. Plavšić, S. Nikolić N. Trinajstić & D. J. Klein, "Relation between the Wiener Index and the Schultz Index for Several Classes of Chemical Graphs", *Croatica Chemica Acta* **66** (1993) 345–353.
174. D. Bonchev, X. Liu & D. J. Klein, "Weighted Self-Returning Walks for Structure-Property Correlations", *Croatica Chemica Acta* **65** (1993) 141–150.
175. D. J. Klein, "Graphitic polymer strips with edge states", *Chemical Physics Letters* **217** (1994) 261–265.
176. A. T. Balaban, D. J. Klein & C. A. Folden, "Diamond-graphite Hybrids", *Chemical Physics Letters* **217** (1994) 266–270.
177. D. Bonchev, A. T. Balaban, X. Liu & D. J. Klein, "Molecular Cyclicity and Centricity of Polycyclic Graphs. I. Cyclicity Based on Resistance Distances and Reciprocal Distances", *International Journal of Quantum Chemistry* **50** (1994) 1–20.
178. A. T. Balaban, D. J. Klein & X. Liu, "Graphitic Cones", *Carbon* **32** (1994) 357–359.
179. D. J. Klein, "Elemental Benzenoids", *Journal of Chemical Information & Computer Sciences* **34** (1994) 453–459.
180. D. J. Klein, M. Randić, D. Babić & N. Trinajstić, "On Conjugated-Circuit Polynomials", *International Journal of Quantum Chemistry* **50** (1994) 369–384.
181. N. Tyutyulkov, F. Dietz, D. J. Klein, W. A. Seitz & T. G. Schmalz, "The Band Gap of Alternant 1D π -Electron Systems", *International Journal of Quantum Chemistry* **51** (1994) 173–180.
182. D. Babić, N. Trinajstić & D. J. Klein, "A Note on a Variant of the Leapfrog Transformation of Chemical Graphs", *Croatica Chemica Acta* **67** (1994) 37–44.
183. H-Y. Zhu, A. T. Balaban, D. J. Klein & T. P. Živković, "Conjugated Circuit Computations on Two-dimensional Carbon Networks", *Journal of Chemical Physics* **101** (1994) 5281–5292.
184. V. O. Chervanovski, T. G. Schmalz & D. J. Klein, "Real-space Renormalization for Heisenberg Models on Two-dimensional Lattices", *Journal of Chemical Physics* **101** (1994) 5841–5846.
185. X. Liu, D. J. Klein & T. G. Schmalz, "Preferable Fullerenes and Clar-Sextet Cages", *Fullerene Science & Technology* **2** (1994) 405–422.
186. M. Randić, D. J. Klein, H-Y. Zhu, N. Trinajstić & T. P. Živković, "Aromatic Properties of Fully Benzenoid Hydrocarbons" *Fizika A* **3** (1994) 61–75.
187. D. J. Klein & X. Liu, "Elemental Carbon Isomerism", *International Journal of Quantum Chemistry S* **28** (1994) 501–523.
188. H-Y. Zhu & D. J. Klein, "Conjugated Circuits for Polymers", *Communications in Mathematical Chemistry* **31** (1994) 205–224.
189. M. Randić, D. J. Klein, H-Y. Zhu, N. Trinajstić & T. P. Živković, "Comparative Study of Large Molecules." *Theoretica Chimica Acta* **90** (1995) 1–26.
190. D. J. Klein & N. H. March, "Similarity Relations and Critical Constants of Heavy Fluid Alkali Metals", *Physics & Chemistry of Liquids* **28** (1994) 207–209.
191. D. J. Klein, I. Lukovits & I. Gutman, "On the Definition of the Hyper-Wiener Index for Cycle-Containing Structures", *Journal of Chemical Information & Computer Sciences* **35** (1995) 50–52.
192. H-Y. Zhu, D. J. Klein, W. A. Seitz & N. H. March, "BN-

- Alternants: Boron Nitride Cages and Polymers", *Inorganic Chemistry* **34** (1995) 1377–1383.
193. A. T. Balaban, H. Zhu & D. J. Klein, "Fullero-Polycoronands", *Fullerene Science and Technology* **3** (1995) 133–150.
 194. T. P. Živković, M. Randić, D. J. Klein, H.-Y. Zhu & N. Trinajstić, "Analytical Approach to Very Large Benzenoid Polymers", *Journal of Computational Chemistry* **16** (1995) 517–526.
 195. N. Trinajstić, M. Randić, D. J. Klein, D. Babić & Z. Mihalić, "On Mathematical Properties of Buckminsterfullerene", *Croatica Chemica Acta* **68** (1995) 241–267.
 196. A. T. Balaban, X. Liu, D. J. Klein, D. Babić, T. G. Schmalz, W. A. Seitz, and M. Randić, "Graph Invariants for Fullerenes", *Journal of Chemical Information & Computer Sciences* **35** (1995) 396–404.
 197. D. Babić, A. T. Balaban and D. J. Klein, "Nomenclature and Coding of Fullerenes", *Journal of Chemical Information & Computer Sciences* **35** (1995) 515–526.
 198. H.-Y. Zhu and D. J. Klein, "Tetrahedral-symmetry tetrahydrofullerenes", *Journal of Molecular Structure* **338** (1995) 11–23.
 199. D. J. Klein, "Algebraic Techniques for Group Theory", pages 1–35 in *Chemical Group Theory*, ed. D. Bonchev and D.H. Rouvray (Gordon & Breach, NY, 1995).
 200. A. T. Balaban, D. Babić, and D. J. Klein, "W. R. Hamilton", *Journal of Chemical Education* **72** (1995) 693–698.
 201. D. J. Klein and N. H. March, "Electron Density in Chemically Bonded Materials and the Chemical Network Model", *Journal of Molecular Structure* **337** (1995) 257–264.
 202. D. J. Klein, A. Graovac, Z. Mihalić & N. Trinajstić, "Excitation Spectra for Degenerate Rearrangements", *Journal of Molecular Structure* **341** (1995) 157–164.
 203. N. H. March, M. P. Tosi, and D. J. Klein, "Coordination-dependent equations of state and pair potentials for cold metal crystals", *Physical Review B* **52** (1995) 9115–9116.
 204. D. J. Klein & N. H. March, "Perfect pairing, natural orbitals, and relations between first- and second-order density matrices", *Journal of Molecular Structure (TheoChem)* **358** (1995) 151–158.
 205. A. T. Balaban, W.A. Seitz & D.J. Klein, "Reversed 'Inverse Superatoms' (Double Fullerene-type Systems)", *Bulletin Societe Chimie Belgique* **104** (1995) 525–530.
 206. D. J. Klein, "Similarity and Dissimilarity in Posets", *Journal of Mathematical Chemistry* **18** (1995) 321–348.
 207. M. A. Garcia-Bach & D. J. Klein, "Cluster-expansion Representation", *Journal of Physics A* **29** (1996) 103–114.
 208. A. T. Balaban, T.G. Schmalz, H.Y. Zhu & D. J. Klein, "Generalizations of the Stone-Wales rearrangement for cage compounds, including fullerenes", *Journal of Molecular Structure (TheoChem)* **363** (1996) 291–302.
 209. D. J. Klein & H.-Y. Zhu, "Resonance in Elemental Benzenoids", *Discrete Applied Mathematics* **67** (1996) 157–173.
 210. H.-Y. Zhu, D. J. Klein & I. Lukovits, "Extensions of the Wiener Number", *Journal of Chemical Information & Computer Science* **36** (1996) 420–428.
 211. H. Zhu & D. J. Klein, "Graph-Geometric Invariants for Molecular Structures", *Journal of Chemical Information & Computer Sciences* **36** (1996) 1067–1075.
 212. A. T. Balaban, D. J. Klein & W. A. Seitz, "Holes in Diamond or Carbon Nitride Lattices", *International Journal of Quantum Chemistry* **60** (1996) 1065–1068.
 213. D. J. Klein & P. G. Mezey, "T-hull relations for shape envelopes of molecular contours", *Theoretica Chimica Acta* **94** (1996) 177–182.
 214. A. T. Balaban, W. A. Seitz & D. J. Klein, "Covalently-bonded 'onion type' double fullerene carbon cages", *Fullerene Science & Technology* **4** (1996) 467.
 215. A. T. Balaban, T. P. Živković, D. J. Klein & T. G. Schmalz, "Reaction graphs for rearrangements of pentagonal-bipyramidal complexes", *Journal of Molecular Structure (TheoChem)* **389** (1997) 265–277.
 216. D. J. Klein, M. Randić, D. Babić, B. Lučić, S. Nikolić & N. Trinajstić, "Hierarchical Orthogonalization of Descriptors", *International Journal of Quantum Chemistry* **63** (1997) 215–222.
 217. H. Zhu, T. G. Schmalz & D. J. Klein, "Alternant Boron Nitride Cages: A Theoretical Study", *International Journal of Quantum Chemistry* **63** (1997) 393–401.
 218. A. T. Balaban & D. J. Klein, "Local Interconversions between Graphite and Diamond Structures", *Carbon* **35** (1997) 247–251.
 219. M. Randić, D. J. Klein, S. El-Basil & P. Calkins, "Resonance in Large Benzenoid Hydrocarbons", *Croatica Chemica Acta* **69** (1996) 1639–1660.
 220. D. J. Klein & H. Zhu, "All-Conjugated Carbon Species", pp. 297–341 in: *From Chemical Topology to Three-Dimensional Geometry*, A. T. Balaban (Ed.) (Plenum Press, New York, 1997).
 221. D. J. Klein, "Graph Geometry, Graph Matrices, and Wiener", *Communications in Mathematical Chemistry (MATCH)* **35** (1997) 7–27.
 222. D. J. Klein & D. Babić "Partial Orderings in Chemistry", *Journal of Chemical Information & Computer Science* **37** (1997) 656–671.
 223. H.-Y. Zhu & D. J. Klein, "Buckyball Superpolyhedra", *Croatica Chemica Acta* **70** (1997) 519–536.
 224. M. A. Garcia-Bach, R. Valenti & D. J. Klein, "Spin Peierls vs. Peierls distortions in a family of conjugated polymers", *Physical Review B* **56** (1997) 1751–1761.
 225. D. J. Klein, H.-Y. Zhu, R. Valenti & M. A. Garcia-Bach, "Many-Body Valence-Bond Theory", *International Journal of Quantum Chemistry* **65** (1997) 421–438.
 226. D. J. Klein, "Inter-Relations between VB & MO Theories for Organic Π -Networks", pp. 33–50 in: *Theoretical Organic Chemistry, Vol 5*, C. Parkanyi (Ed.) (Elsevier, Amsterdam, 1997).
 227. N. H. March & D. J. Klein, "Ising, Heisenberg and Hubbard Models in Relation to Insulating and Metallic Ferro- and Antiferro-magnets", pp. 1–13 in: *Theory of Spin Lattices & Lattice Gauge Models*, J. W. Clark & M. L. Ristig (Eds.) (Springer-Verlag, Berlin, 1997).
 228. H.-Y. Zhu, D. J. Klein, T. G. Schmalz, A. Rubio & N. H. March, "Geometric Boundary Effects on the Electronic Properties of Finite Carbon Nanotubes", *Journal of Physics & Chemistry of Solids* **59** (1998) 417–423.
 229. D. J. Klein, N. H. March & A. K. Theophilou, "Form of spinless first- & second-order density matrices in atoms & molecules, derived from eigenfunctions of S_2 & S_z ", *Journal of Mathematical Chemistry* **21** (1997) 261–272.
 230. C. Amovilli, N. H. March, T. G. Schmalz & D. J. Klein, "Thomas-Fermi theory of an inhomogeneous electron liquid generalized to incorporate density gradients", *Physics & Chemistry of Liquids* **36** (1998) 91–103.
 231. D. J. Klein & H.-Y. Zhu, "Distances & Volumina for Graphs", *Journal of Mathematical Chemistry* **23** (1998) 179–195.
 232. N. Flocke, T. G. Schmalz & D. J. Klein, "Variational resonance valence bond study on the ground state of C_{60} using the Heisenberg model", *Journal of Chemical Physics* **109** (1998) 873–880.
 233. L. Bytautas & D. J. Klein, "Symmetry Aspects of Nonrigid Molecules & Transition Structures in Chemical Reactions", *Internation-*

- tional Journal of Quantum Chemistry* **70** (1998) 205–217.
234. H.-Y. Zhu, D. J. Klein, N. H. March & A. Rubio, "Small Band-Gap Graphitic CBN Layers", *Journal of Physics & Chemistry of Solids* **8** (1998) 1303–1308.
 235. L. Bytautas & D. J. Klein, "Chemical Combinatorics for Alkane-Isomer Enumeration and More", *Journal of Chemical Information and Computer Sciences* **38** (1998) 1063–1078.
 236. T. G. Schmalz, N. Flocke & D. J. Klein, "Valence Bond Study of Fullerenes Using the Heisenberg Model", *Recent Advances in the Chemistry & Physics of the Fullerenes & Related Materials* **6** (1998) 47–59.
 237. D. J. Klein & I. Gutman, "Wiener-Number-Related Sequences", *Journal of Chemical Information & Computer Sciences* **39** (1999) 534–536.
 238. D. J. Klein, "Topo-Graphs, Embeddings, and Molecular Structure" pp. 39–83 in: *Mathematical Chemistry, vol. 4 - Chemical Topology*, D. Bonchev & D.H. Rouvray (Eds.) (Gordon and Breach Pub., NY, 1999).
 239. D. J. Klein, "Advances in Many-Body Valence-Bond Theory", pp. 403–420 in: *Pauling's Legacy: Modern Modelling of the Chemical Bond*, Z. B. Maksic & W. J. Orville-Thomas (Eds.) (Elsevier, Amsterdam, 1999)
 240. D. J. Klein, "Resonating Valence Bond Theory and Magnetic Properties", pp. 41–59 in: *Magnetic Properties of Organic Materials*, P. M. Lahti (Ed.) (Marcel Dekker, NY, 1999).
 241. L. Bytautas & D. J. Klein, "Isomer combinatorics for acyclic conjugated polyenes: enumeration and beyond", *Theoretical Chemistry Accounts* **101** (1999) 371–387.
 242. D. J. Klein & L. Bytautas, "Graphitic Edges and Unpaired π -Electron Spins", *Journal of Physical Chemistry A* **103** (1999) 5196–5210.
 243. D. J. Klein, T.G. Schmalz & L. Bytautas, "Chemical Sub-Structural Cluster Expansions for Molecular Properties", *SAR & QSAR in Environmental Research* **10** (1999) 131–156.
 244. L. Bytautas & D.J. Klein, "Formula Periodic Table for Acyclic Hydrocarbon Isomer Classes: Combinatorially Averaged Graph Invariants", *Physical Chemistry - Chemical Physics* **1** (1999) 5565–5572.
 245. N. H. March, D. J. Klein, A. K. Ray & X. Wu, "Sin Clusters: Surface Energy Considerations for Large n and All-Electron Hartree-Fock Calculations for n=45", *International Journal of Quantum Chemistry* **75** (1999) 829–838.
 246. C. Amovilli, N. H. March, T. G. Schmalz, G. E. Hite & D. J. Klein, "Inhomogeneous Electron Liquid: Differential Equation Satisfied by Diagonal Element of Coulomb Bound s-State Green Function", *Physics & Chemistry of Liquids* **37** (1999) 475–478.
 247. L. Bytautas & D. J. Klein, "Alkane Isomer Combinatorics: Stereostructure Enumeration and Graph-Invariant and Molecular-Property Distributions", *Journal of Chemical Information & Computer Sciences* **39** (1999) 803–818.
 248. N. Flocke, T. G. Schmalz & D. J. Klein, "Ground and Excited Hubbard States for Buckminsterfullerene with Uniform and Alternating Bond Strengths", *Journal of Chemical Physics* **112** (2000) 8233–8240.
 249. A. T. Balaban, D. J. Klein & W. A. Seitz, "Large 'Pillow' Fullerenes as Graphite without Dangling Bonds", *Fullerene Science & Technology* **8** (2000) 249–265.
 250. L. Bytautas & D. J. Klein, M. Randić & T. Pisanski, "Foldedness in Linear Polymers: A Difference Between Graphical and Euclidean Distances", *DIMACS Series in Discrete Mathematics & Theoretical Computer Science* **51** (2000) 39–61.
 251. L. Bytautas & D. J. Klein, "Mean Wiener Numbers and Other Mean Extensions for Alkane Trees", *Journal of Chemical Information & Computer Science* **40** (2000) 471–481.
 252. T. P. Živković, D. J. Klein & T. G. Schmalz, "Covalent Isoresonance", *Polycyclic Aromatic Compounds* **13** (2000) 457–471.
 253. T. P. Živković, T. G. Schmalz & D. J. Klein, "Isoresonant Benzenoids", *Polycyclic Aromatic Compounds* **18** (2000) 13–24.
 254. L. Bytautas, D. J. Klein & T. G. Schmalz, "All acyclic hydrocarbons: formula periodic table and property overlap plots via chemical combinatorics", *New Journal of Chemistry* **24** (2000) 329–336.
 255. L. Bytautas & D. J. Klein, "Formula Periodic Table for the Isomer Classes of Acyclic Hydrocarbons - Enumeration and Asymptotic Characters", *Croatica Chemica Acta* **73** (2000) 331–357.
 256. N. H. March, C. Amovilli & D. J. Klein, "The wave-function when antiparallel spin electrons coincide and its relation to the ground-state electron density in the Hookean atom", *Chemical Physics Letters* **325** (2000) 645–647.
 257. D. J. Klein, "Prolegomenon on Partial Orderings in Chemistry", *Communications in Mathematical Chemistry (MATCH)* **42** (2000) 7–21.
 258. D. J. Klein & L. Bytautas, "Directed Reaction Graphs as Posets", *Communications in Mathematical Chemistry (MATCH)* **42** (2000) 261–290.
 259. J. Szucs & D. J. Klein, "Regular affine tilings and regular maps on a flat torus", *Discrete Applied Mathematics* **105** (2000) 225–237.
 260. O. Ivanciuc, T. Ivanciuc, D. J. Klein, W. A. Seitz & A. T. Balaban, "Quantitative Structure- Retention Relationships for Gas Chromatographic Retention Indices of Alkylbenzenes with Molecular Graph Descriptors", *SAR & QSAR in Environmental Research* **11** (2001) 419–452.
 261. D. Babić, D. J. Klein & T. G. Schmalz, "Curvature matching and strain relief in bucky-tori: usage of sp³-hybridization and nonhexagonal rings", *Journal of Molecular Graphics and Modelling* **19** (2001) 223–231.
 262. O. Ivanciuc, T. Ivanciuc, D. J. Klein, W. A. Seitz & A. T. Balaban, "Wiener Index Extension by Counting Even/Odd Graph Distances", *Journal of Chemical Information & Computer Science* **41** (2001) 536–549.
 263. O. Ivanciuc, T. Ivanciuc & D. J. Klein, "Quantitative Structure-Property Relationships Generated with Optimizable Even/Odd Wiener Polynomial Descriptors", *SAR & QSAR in Environmental Research* **12** (2001) 1–16.
 264. D. J. Klein & N. H. March, "Molecular Magnetism via Resonating Valence Bonds for Conjugated Radicals and Selected Transition Metal Complexes", *International Journal of Quantum Chemistry* **85** (2001) 327–344.
 265. A. Peeters, C. Van Alsenoy, N. H. March, D. J. Klein & V. E. Van Doren, "Boron B12 Cluster Embedded in Graphitic Fragments", *Journal of Physical Chemistry B* **105** (2001) 10546–10553.
 266. L. Bytautas, D. Bonchev & D. J. Klein, "On the Generation of Mean Wiener Numbers of Thorny Graphs", *Communications in Mathematical Chemistry (MatCh)* **44** (2001) 31–40.
 267. O. Ivanciuc, T. Ivanciuc & D. J. Klein, "Intrinsic Graph Distances Compared to Euclidean Distances for Correspondent Graph Embedding", *Communications in Mathematical Chemistry (MatCh)* **44** (2001) 251–278.
 268. S. B. Santra, W. A. Seitz & D. J. Klein, "Directed self-avoiding walks in random media", *Physical Review E* **63** (2001) 067101-1–4.
 269. O. Ivanciuc, L. Bytautas & D. J. Klein, "Mean Field Resonating-

- Valence-Bond Theory for Unpaired Pi-Electrons in Benzenoid Carbon Species", *Journal of Chemical Physics* **116** (2002) 4736–4748.
270. O. Ivanciuc & D. J. Klein, "Computing Wiener-Type Indices for Virtual Combinatorial Libraries Generated from Heteroatom-Containing Building Blocks", *Journal of Chemical Information & Computer Sciences* **42** (2002) 8–22.
271. D. J. Klein, R. P. Hurst & N. H. March, "Quantum-mechanical model relating negative-ion polarizabilities in free space and in an ionic crystal", *Journal of Physics & Chemistry of Solids* **63** (2002) 287–294.
272. D. J. Klein & O. Ivanciuc, "Graph Cyclicity, Excess Conductance & Resistance Deficit", *Journal of Mathematical Chemistry* **30** (2002) 271–287.
273. D. J. Klein, "Topo-combinatoric categorization of quasi-local graphitic defects", *Physical Chemistry - Chemical Physics* **4** (2002) 2099–2110.
274. O. Ivanciuc, D. J. Klein & L. Bytautas, "Unpaired π -spin density in defected graphite", *Carbon* **40** (2002) 2063–2083.
275. O. Ivanciuc & D. J. Klein, "Building Block Computation of Wiener-Type Indices for the Virtual Screening of Combinatorial Libraries", *Croatica Chemica Acta* **75** (2002) 577–601.
276. D. Bonchev & D. J. Klein, "On the Wiener Number of Thorn Trees, Stars & Rods", *Croatica Chemica Acta* **75** (2002) 613–620.
277. D. J. Klein, "Resistance-Distance Sum Rules", *Croatica Chemica Acta* **75** (2002) 633–649.
278. D. J. Klein, D. Babić & N. Trinajstić, "Enumeration in Chemistry", *Chemical Modelling - Applications & Theory* **2** (2002) 56–95.
279. A. T. Balaban & D. J. Klein, "Co-authorship, rational Erdos numbers, and resistance distances in graphs", *Scientometrics* **55** (2002) 59–70.
280. D. Babić, D. J. Klein, I. Lukovits, S. Nikolić & N. Trinajstić, "Resistance-Distance Matrix: A Computational Algorithm & Its Application", *International Journal of Quantum Chemistry* **90** (2002) 166–176.
281. D. J. Klein, "Resonating Valence-Bond Theories for Carbon π -Networks and Classical/Quantum Connections", pp. 233–287 in: *Valence Bond Theory*, D. L. Cooper (Ed.) (Elsevier, Amsterdam, 2002).
282. D. J. Klein, "Graph Geometry via Metrics", pp. 292–317 in: *Topology in Chemistry*, D. H. Rouvray & R. B. King (Eds.) (Horwood Pub., Chichester, 2002).
283. A. Misra & D. J. Klein, "Characterization of Cyclo-Polyphenacenes", *Journal of Chemical Information & Computer Science* **42** (2002) 1171–1175.
284. D. J. Klein & A. Misra, "Topological Isomer Generation & Enumeration: Application for Polyphenacenes", *Communications in Mathematical & Computer Chemistry (MatCh)* **46** (2002) 45–69.
285. Jian Wu, T. G. Schmalz & D. J. Klein, "An extended Heisenberg model for conjugated hydrocarbons", *Journal of Chemical Physics* **117** (2002) 9977–9982.
286. C. Amovilli, I. A. Howard, D. J. Klein & N. H. March, "Dependence of the pi-electron eigenvalue sum on the number of atoms in almost spherical C cages", *Physical Review A* **66** (2002) 013210-1–5.
287. I. A. Howard, N. H. March & D. J. Klein, "Edge confinement of a two-dimensional electron gas and its relevance to the electron density near a vacancy defect in graphite", *Journal of Mathematical Chemistry* **32** (2002) 31–37.
288. Jian Wu, D. J. Klein & T. G. Schmalz, "Computation on Symmetry-Invariant Bases", *International Journal of Quantum Chemistry* **94** (2003) 7–22.
289. D. J. Klein, "Partitioning of Wiener-type indices, especially for trees", *Indian Journal of Chemistry* **42A** (2003) 1264–1269.
290. Jian Wu, T. G. Schmalz & D. J. Klein, "Semiempirical Valence-Bond Resonance Energies for Alternant Conjugated Hydrocarbons Containing Four-Membered Rings", *International Journal of Quantum Chemistry* **95** (2003) 455–460.
291. A. Misra, D. J. Klein, S. N. Datta & N. H. March, "Internal Energy and Magnetic Moment of Three-Dimensional Ferromagnets", *International Journal of Quantum Chemistry* **95** (2003) 451–454.
292. D. J. Klein, "Quasilocal Defects in Regular Planar Networks; Categorization for Molecular Cones", *International Journal of Quantum Chemistry* **95** (2003) 600–616.
293. Jian Wu, T. G. Schmalz & D. J. Klein, "An extended Heisenberg model for conjugated hydrocarbons. II. Kekule basis", *Journal of Chemical Physics* **119** (2003) 11011–11016.
294. N. H. March, A. T. Balaban, F. E. Leys, D. J. Klein & W. A. Seitz, "Regularities in melting points of lithium halides: Is LiH anomalous?", *Physics & Chemistry of Liquids* **41** (2003) 303–308.
295. D. J. Klein, "Graph Theoretically Formulated Electronic-Structure Theory", *Internet Electronic Journal of Molecular Design* **2** (2003) 814–834.
296. T. Ivanciuc & D. J. Klein, "Parameter-Free Structure-Property Correlation via Progressive Reaction Posets for Substituted Benzenes", *Journal of Chemical Information & Computer Sciences* **44** (2004) 610–617.
297. D. J. Klein & A. Misra, "Minimally Kekulenoid Pi-Networks and Reactivity for Acyclics", *Croatica Chemica Acta* **77** (2004) 179–191.
298. E. Kirby, D. J. Klein, P. Pollack, R. B. Mallion & H. Sachs, "A Theorem for Counting Spanning Trees in General Chemical Graphs and Its Particular Application to Toroidal Fullerenes", *Croatica Chemica Acta* **77** (2004) 263–278.
299. D. Babić, D. J. Klein, J. V. Knop & N. Trinajstić, "Combinatorial Chemical Enumeration", *Chemical Modelling - Applications & Theory* **3** (2004) 126–170.
300. L. Pogliani, D. J. Klein & A. T. Balaban, "The Number Two and the Intriguing Dualism of Nature, Scientific Curiosity and Everyday Concepts", *Communications in Mathematical & Computer Chemistry* **51** (2004) 213–240.
301. G. G. N. Angilella, F. Bartha, G. Bogar, D. J. Klein, N. H. March, R. Pucci & F. Siringo, "Electronic structure of condensed phases of some light elements subjected to high pressure", *Recent Research Developments in Physics* **4** (2004) 861–875.
302. D. J. Klein, J. Palacios, M. Randić & N. Trinajstić, "Random Walks and Chemical Graph Theory", *Journal of Chemical Information & Computer Science* **44** (2004) 1517–1520.
303. A. Misra, A. Ayuela, D. J. Klein & N. H. March, "Magnetically ordered materials: relation between internal energy, magnetization and applied field", *Physics Letters A* **329** (2004) 396–401.
304. T. Morikawa, S. Narita & D. J. Klein, "A classical Valence Bond view of cylinder-shaped and fully benzenoid-like polyarenes (polycyclic aromatic hydrocarbons) of large size", *Polycyclic Aromatic Compounds* **24** (2004) 195–206.
305. D. Babić, T. Doslić, D. J. Klein & A. Misra, "Kekulenoid Addition Patterns for Fullerenes", *Bulletin of the Chemical Society of Japan* **77** (2004) 2003–2010.
306. T. Morikawa, S. Narita & D. J. Klein, "Molecules-in-Molecule Estimation of the Extent of Localization of Kekulean Substructures in Polycyclic Aromatic Hydrocarbons", *Journal of Chemi-*

- cal Information & Computer Science* **44** (2004) 1891–1896.
307. D. J. Klein & N. H. March, "The role of disclinations in two phase changes induced by temperature and pressure in crystalline solids: melting and the brittle-ductile transition", *Physics & Chemistry of Liquids* **42** (2004) 545–550.
 308. I. A. Howard, D. J. Klein, N. H. March, C. Van Alsenoy, S. Suhai, Z. Janosvalfi & A. Nagy, "Change in Electronic Structure of Polyenes Due to Interaction with Polyacenes and with Graphitic Strips", *Journal of Physical Chemistry B* **108** (2004) 14870–14875.
 309. T. Došlić & D. J. Klein, "Splinoïd interpolation on finite posets", *Journal of Computational & Applied Mathematics* **177** (2005) 175–185.
 310. D. Vukićević & D. J. Klein, "Characterization of distribution of pi-electrons amongst benzenoid rings for Randić's 'algebraic' Kekule structures", *Journal of Mathematical Chemistry* **37** (2005) 163–170.
 311. L. L. Griffin, Jian Wu, D. J. Klein, T. G. Schmalz & L. Bytautas, "Scaling Behavior of Ground-State Energy Cluster Expansion for Linear Polyenes", *International Journal of Quantum Chemistry* **102** (2005) 387–397.
 312. A. T. Balaban, D. J. Klein & O. Ivanciuc, "Large 'Pillow' Fullerenes Hydrogenated at the Inter-sheet 'Seam'", *Fullerenes, Nanotubes & Carbon Nanostructures* **13** (2005) 109–129.
 313. T. Morikawa, S. Narita & D. J. Klein, "Molecular electric conductance and long-bond structure counting for conjugated-carbon nano-structures", *Chemical Physics Letters* **402** (2005) 554–558.
 314. T. Morikawa & D. J. Klein, "Quantification of Pi-Electron Capacity of Kekulean Substructures in Benzenoid Hydrocarbons", *Polycyclic Aromatic Compounds* **25** (2005) 129–140.
 315. A. T. Balaban, D. J. Klein, N. H. March & C. C. Matthai, "Transport and Thermodynamic properties in low melting point ionic liquids related to n-alkyl chain length", *Physics & Chemistry of Liquids* **43** (2005) 403–407.
 316. A. T. Balaban, D. J. Klein, N. H. March, M. P. Tosi & M. Ausloos, "Phase-Transition Regularities in Critical Constants, Fusion Temperatures and Enthalpies of Chemically Similar Chainlike Structures", *ChemPhysChem* **6** (2005) 1–5.
 317. T. Ivanciuc, O. Ivanciuc & D. J. Klein, "Posetic quantitative superstructure/activity relationships (QSSARs) for chlorobenzenes", *Journal of Chemical Information & Modeling* **45** (2005) 870–879.
 318. D. J. Klein & T. Ivanciuc, "Mean-field resonance-theoretic view of Benzenoid networks" *Arhivoc* **2005** (2005) 292–307.
 319. D. J. Klein & A. T. Balaban, "The Eight Classes of Positive-Curvature Graphitic Nanocones", *Journal of Chemical Information & Modeling* **46** (2006) 307–320.
 320. T. Ivanciuc, O. Ivanciuc & D. J. Klein, "Modeling the bioconcentration factors and bioaccumulation factors of polychlorinated biphenyls with posetic quantitative superstructure/activity relationships (QSSAR)", *Molecular Diversity* **10** (2006) 133–145.
 321. Xiao-Feng Guo, D. J. Klein, W. Yan & Y.-N. Yeh, "Hyper-Wiener Vector, Wiener Matrix Sequence, and Wiener Polynomial Sequence of a Graph", *International Journal of Quantum Chemistry* **106** (2006) 1756–1761.
 322. T. Ivanciuc, O. Ivanciuc & D. J. Klein, "Prediction of Environmental Properties for Chlorophenols with posetic Quantitative Super-Structure/Property Relationships (QSSAR)", *International Journal of Molecular Sciences* **7** (2006) 358–374.
 323. A. T. Balaban & D. J. Klein, "Is chemistry 'The Central Science'? How are different sciences related? Co-citations, reductionism, emergence, and posets", *Scientometrics* **69** (2006) 615–637.
 324. D. J. Klein & N. H. March, "Spin-polarized electron (hole) liquids: Are pi-electrons in metal-benzene sandwiches or injected carriers in C-doped BN nanotubes candidates", *J. Phys. & Chemistry of Liquids* **44** (2006) 337–341.
 325. D. J. Klein & T. Ivanciuc, "Directed Reaction Graphs as Posets", pp. 35–60 in: *Partial Order in Environmental Science and Chemistry*, R. Bruggemann & L. Carlsen (Eds.) (Springer Verlag, Berlin, 2006).
 326. T. Ivanciuc, D. J. Klein & O. Ivanciuc, "Posetic Cluster Expansion for Substitution-Reaction Networks and Application to Methylated Cyclobutanes", *Journal of Mathematical Chemistry* **41** (2007) 355–379.
 327. R. Pepper & D. J. Klein, "Some Theorems About the Randić Connectivity Index", *Communications in Mathematical & Computer Chemistry (MATCH)* **58** (2007) 359–364.
 328. A. Ayuela, D. J. Klein & N. H. March, "Sublattice magnetizations in non-zero magnetic field in an antiferromagnetic infinite-range Ising model", *Physics Letters A* **362** (2007) 468–470.
 329. D. J. Klein, T. Došlić & D. Bonchev, "Vertex-Weightings and Distance Moments for Thorny Graphs", *Discrete Applied Mathematics* **155** (2007) 2294–2302.
 330. D. J. Klein & N. H. March, "Is the brittle-ductile transition preceding melting related to 5- and 7-membered ring defects in graphite?", *Physics & Chemistry of Liquids* **45** (2007) 609–613.
 331. A. T. Balaban, D. J. Klein, J. E. Dahl & R. M. K. Carlson, "Molecular Descriptors for Natural Diamondoid Hydrocarbons and Quantitative Structure-Property Relationships for Their Chromatographic Data", *The Open Organic Chemistry Journal* **1** (2007) 13–131.
 332. V. Manero, J. Oliva, L. Serrano-Andres & D. J. Klein, "What is the Limit of Atom Encapsulation for Icosahedral Carboranes?" *Journal of Chemical Theory and Computation* **3** (2007) 1399–1404.
 333. A. T. Balaban, D. J. Klein & N. H. March, "Aqueous solutions of a "green" ionic liquid and of lithium chloride compared and contrasted", *Physics & Chemistry of Liquids* **45** (2007) 597–601.
 334. A. Ayuela, N. H. March & D. J. Klein, "Optimized Geometry of the Cluster Gd₂O₃ and Proposed Antiferromagnetic Alignment of f-Electron Magnetic Moment", *Journal of Physical Chemistry A* **111** (2007) 10162–10165.
 335. D. J. Klein, "Defected/decorated benzenoid/graphitic nanostructures", *Pure & Applied Chemistry* **80** (2008) 1399–1414.
 336. J. I Burgos, L. Serrano-Andres, J. M. Oliva & D. J. Klein, "On the Effect of Radical Character, Substitution and Atom Encapsulation on the Volume of Icosahedral (Car)boranes", *Afinidad* **65** (2008) 32–38.
 337. L. Serrano-Andres, D. J. Klein, P. v. R. Schleyer & J. M. Oliva, "What Electronic Structures and Geometries of Carborane Mono- and ortho-, meta- & para-Diradicals are Preferred?", *Journal of Chemical Theory and Computation* **4** (2008) 1338–1347.
 338. D. J. Klein & N. H. March, "Critical exponents in D dimensions for the Ising model, subsuming Zhang's proposals for D = 3", *Physics Letters A* **372** (2008) 5052–5053.
 339. D. J. Klein, T. Ivanciuc, A. Ryzhov & O. Ivanciuc, "Combinatorics of Reaction-Network Posets", *Combinatorial Chemistry and High Throughput Screening* **11** (2008) 723–733.
 340. A. T. Balaban, N. H. March & D. J. Klein, "Melting points and other properties of ionic liquids, with emphasis on the pressure dependence", *Physics & Chemistry of Liquids* **46** (2008) 682–686.
 341. A. T. Balaban, N. H. March & D. J. Klein, "Relation of surface tension to compressibility at room temperature and wetting index

- also involving viscosity for 22 organic liquids", *Physics & Chemistry of Liquids* **47** (2009) 1–4.
342. J. Oliva, D. J. Klein, P. V. R. Schleyer & L. Serrano-Andres, "Design of Carborane Molecular Architectures with Electronic Structure Computations: From Endohedral and Polyradical Systems to Multidimensional Networks", *Pure & Applied Chemistry* **81** (2009) 719–729.
343. D. J. Klein, A. Ryzhov & V. Rosenfeld, "Permutational Isomers on a Molecular Skeleton with Neighbor-Excluding Ligands", *Journal of Mathematical Chemistry* **45** (2009) 892–909.
344. A. T. Balaban, K. Chilikamari & D. J. Klein, "Protochirons and protohelices", *Journal of Mathematical Chemistry* **45** (2009) 725–747.
345. A. Misra, D. J. Klein & T. Morikawa, "Clar Theory for Molecular Benzenoids", *Journal of Physical Chemistry A* **113** (2009) 1151–1158.
346. A. T. Balaban, D. J. Klein, and N. H. March, "Modelling the structure of the water molecule under both local environmental constraints and explosive conditions", *Physics & Chemistry of Liquids* **47** (2009) 471–473.
347. D. J. Klein, N. H. March & J. A. Alonso, "Fractal network dimension determining the relation between the strength of bulk metallic glasses and the glass transition temperature", *Applied Physics Letters* **95** (2009) 021909-1–3.
348. D. J. Klein, V. Rosenfeld & G. Restrepo, "Stereo-Chemical Combinatorics & Beyond", pp. 421–424 in: *Computational Methods in Science and Engineering, AIP Conference Proceedings Vol. 1148*, T. E. Simos & G. Maroulis (Eds.) (AIP, NY, 2009).
349. A. T. Balaban & D. J. Klein, "Claromatic Carbon Nano-Structures", *Journal of Physical Chemistry C* **113** (2009) 19123–19134.
350. A. Misra, T. G. Schmalz & D. J. Klein, "Clar Theory for Radicaloid Benzenoids", *Journal of Chemical Information & Modelling* **49** (2009) 2670–2676.
351. J. M. Oliva, L. Serrano-Andres, D. J. Klein, P. V. R. Schleyer & J. Michl, "Design of Carborane Molecular Architectures via Electronic Structure Computations", *International Journal of Photoenergy* **2009** (2009) 292393-1–9.
352. N.H. March, D.J. Klein, G.G.N. Angilella, R. Pucci & J.A. Alonso, "High-pressure behaviour of crystalline silane compared with that for SnH₄", *Phase Transitions* **82** (2009) 247–250.
353. D. J. Klein & V. Rosenfeld, "The Degree-Product Index of Naurumi & Katayama", pp. 79–90 in: *Novel Molecular Structure Descriptors – Theory and Applications II*, B. Furtula & I. Gutman (Eds.) (Univ. Kragujevac, Kragujevac, 2010).
354. W. Yang, F. Zhang & D. J. Klein, "Benzenoid Links", *Journal of Mathematical Chemistry* **47** (2010) 457–476.
355. D. Bhattacharya, S. Shil, A. Misra & D. J. Klein, "Intramolecular ferromagnetic coupling in bis-oxoverdazyl and bis-thioxoverdazyl diradicals with polyacene spacers", *Theoretical Chemistry Accounts* **127** (2010) 57–67.
356. D. J. Klein, "Centrality Measure in Graphs", *Journal of Mathematical Chemistry* **47** (2010) 1209–1223.
357. D. J. Klein & J. Oliva, "Composite System Models", *International Journal of Quantum Chemistry* **110** (2010) 2784–2800.
358. D. J. Klein, "Vector Representations of Kekule Structures of Benzenoids", *Slovenica Chemica Acta* **57** (2010) 591–596.
359. D. J. Klein & V. Rosenfeld, "The Degree-Product Index of Naurumi & Katayama", *Communications in Mathematical and Computer Chemistry (MATCH)* **64** (2010) 607–618.
360. V. Rosenfeld & D. J. Klein, "Implications of Sense/Antisense Nucleic-Acid Codons on Amino-Acid Counts", *Studia Universitatis Babeş-Bolyai* **55** (2010) 167–176.
361. V. Rosenfeld & D. J. Klein, "Cyclic Nucleotide Sequences Codonically Invariant under Frame Shifting", *Studia Universitatis Babeş-Bolyai* **55** (2010) 177–182.
362. J. Nava, V. Kreinovich, G. Restrepo & D. J. Klein, "Discrete Taylor Series as a Simple Way to Predict Properties of Chemical Substances like Benzenes and Cubanes", *Journal of Uncertain Systems* **4** (2010) 270–290.
363. D. J. Klein, "Spin-Free Quantum Electronic Structure: Its Second Quantization and Para-Fermionics", *International Journal of Quantum Chemistry* **111** (2011) 76–95.
364. T. Ivanciuc, O. Ivanciuc & D. J. Klein, "Network-QSAR with Reaction Poset Quantitative Superstructure-Activity Relationships (QSSAR) for PCB Chromatographic Properties", *Current Bioinformatics* **6** (2011) 25–34.
365. G. Restrepo, R. Brüggemann & D. J. Klein, "Partially Ordered Sets: Ranking and Prediction of Substances' Properties", *Current Computer-Aided Drug Design* **7** (2011) 133–145.
366. D. J. Klein & V. Rosenfeld, "Phased Graphs and Graph Energies", *Journal of Mathematical Chemistry* **49** (2011) 1238–1244.
367. D. J. Klein & V. Rosenfeld, "Phased Cycles", *Journal of Mathematical Chemistry* **49** (2011) 1245–1255.
368. D. J. Klein & V. Rosenfeld, "Dinormal Graphs", *Journal of Mathematical Chemistry* **49** (2011) 1256–1262.
369. Y. Yang, H. Zhang & D. J. Klein, "New Nordhaus-Gaddum-Type Results for the Kirchhoff index", *Journal of Mathematical Chemistry* **49** (2011) 1587–1598.
370. D. J. Klein & A. T. Balaban, "Clarology for Conjugated Carbon Nano-Structures: Molecules, Polymers, Graphene, Defected Graphene, Fractal Benzenoids, Fullerenes, Nano-Tubes, Nano-Cones, Nano-Tori, etc.", *Open Journal of Organic Chemistry* **5** (2011) 27–61 (Suppl 1-M3).
371. V. O. Cheranovskii, E. V. Ezerskaya, D. J. Klein & Aleksei A. Kravchenko, "Magnetic properties of model non-carbon nanotubes with macroscopic value of ground-state spin", *Journal of Magnetism & Magnetic Materials* **323** (2011) 1636–1642.
372. G. Restrepo & D. J. Klein, "Predicting densities of nitrocubanes using partial orders", *Journal of Mathematical Chemistry* **49** (2011) 1311–1321.
373. V. Rosenfeld, J. Oliva & D. J. Klein, "Enumeration of Carborane Chains", *Monatshefte für Chemie* **143** (2012) 361–364.
374. G. Forte, J. M. Oliva, A. T. Balaban, D. J. Klein & N. H. March, "Modelling X-ray scattering factors from fluids of some fluorinated molecules and related compounds", *Physics & Chemistry of Liquids* (2012) 1-9.
375. V. Rosenfeld, D. J. Klein & J. M. Oliva, "Enumeration of Polycarborane Isomers: especially dicarboranes", *Journal of Mathematical Chemistry* **50** (2012) 2012–2022.
376. R. Kar, A. Misra, N. H. March & D. J. Klein, "Bose–Einstein condensation of magnons in ferromagnetic thin films", *Phase Transitions* **85** (2012) 831–839.
377. D. Babić, D. J. Klein & D. M. Smith, "Staggered Benzenoid Pairs as Potential Spin Coupling Systems", *Communications in Mathematical & Computer Chemistry (MATCH)* **69** (2013) 649–676.
378. V. Rosenfeld & D. J. Klein, "Enumeration of Substitutional Isomers with Restrictive Mutual Positions of Ligands. I. Overall Counts", *Journal of Mathematical Chemistry* **51** (2013) 21–37.
379. V. Rosenfeld & D. J. Klein, "Enumeration of Substitutional Isomers with Restrictive Mutual Positions of Ligands. II. Counts with restrictions on (sub)symmetry", *Journal of Mathematical Chemistry* **51** (2013) 239–264.
380. D. J. Klein & C. E. Larson, "Eigenvalues of Saturated Hydrocar-

- bons", *Journal of Mathematical Chemistry* **51** (2013) 1608–1618.
381. O. Ivanciuc, T. Ivanciuc & D. J. Klein, "Flow Network QSAR for the Prediction of Physicochemical Properties by Mapping an Electrical Resistance Network onto a Chemical Reaction Poset", *Current Computer-Aided Drug Design* **9** (2013) 233–240.
382. D. J. Klein, "Mathematical Chemistry! Is it? And if so, then what is it?", *HYLE – International Journal for Philosophy of Chemistry* **19** (2013) 35–85.
383. Y. Yang & D. J. Klein, "Recursion Relations for Resistance Distance & Its Application", *Discrete Applied Mathematics* **161** (2013) 2702–2715.
384. D. J. Klein & E. Yi, "A Comparison on Metric Dimension of Graphs, Line Graphs, and Line Graphs of the Subdivision Graphs", *European Journal of Pure & Applied Mathematics* **5** (2012) 302–316.
385. A. Panda, S. Vijayakumar, D. J. Klein & A. Ryzhov, "Network of Secondary-Substituted Adamantane Amines", *Journal of Physical Organic Chemistry* **26** (2013) 917–926.
386. D. Bhattacharya, S. Shil, T. Goswami, A. Misra, A. Panda & Douglas J. Klein, "A Theoretical Study on Magnetic Properties of Bis-TEMPO Diradicals with Possible Application", *Computational & Theoretical Chemistry* **1024** (2013) 15–23.
387. B. Mandal & D. J. Klein, "Analytical Eigenspectra of Alternant Edge Weighted Graphs of Linear Chains and Cycles: Some Applications", *Mol. Phys.* (submitted 2013).
388. B. Mandal & D. J. Klein, "Characteristic polynomial followed by trigonometric identity for obtaining analytical eigenspectra of some weighted graphs of linear chains and cycles", *Bulletin of the Chemical Society of Japan* (submitted 2013).
389. D. J. Klein & V. Rosenfeld, "Forcing, Freedom, & Uniqueness in Graph Theory & Chemistry", *Croatica Chemica Acta* (accepted, 2013).
390. D. J. Klein, "Substitution-Reaction Posets & Neatly Graded Posets", *Communications in Mathematical & Computer Chemistry* (submitted, 2013)
391. A. Panda, D. Bhattacharya, A. Misra, & D. J. Klein, "Clar Theory for Polyacenes", (to be submitted 2013).