

**Project: Graph theory and mathematical programming with
applications in chemistry and engineering**

PUBLICATIONS IN 2010

SCIENTIFIC PAPERS

Spectra of graphs

1. D. Cvetković, S.K. Simić, Towards a spectral theory of graphs based on the signless Laplacian, II, *Linear Algebra and Appl.*, 432(2010), 156-166.
2. D. Cvetković, S.K. Simić, Towards a spectral theory of graphs based on the signless Laplacian, III, *Appl. Anal. Discrete Math.*, 4(2010), 156-166.
3. J. Wang, F. Belardo, Q.X. Huang, B. Borovićanin, On the two largest Q-eigenvalues of graphs, *Discrete Mathematics*, 310 (21) (2010), 2858-2866.
4. S.K. Simić, Z. Stanić, On Q-integral (3,s)-semiregular bipartite graphs, *Appl. Anal. Discrete Math.*, 4(2010), 167-174.
5. M. Anđelić, S.K. Simić, Some notes on threshold graphs, *Discrete Math.*, 310(2010), 2241-2248.
6. D. Cvetković, S.K. Simić, Z. Stanić, Spectral determination of graphs whose components are paths and cycles, *Computers and Math. with Appl.*, 59(2010), 3849-3857.
7. F. Belardo, E.M. Li Marzi, S.K. Simić, J. Wang, On the spectral radius of unicyclic graphs with prescribed degree sequence, *Linear Algebra and Appl.*, (432)9(2010), 2323-2334.
8. S.K. Simić, F. Belardo, E.M. Li Marzi, D.V. Tošić, Connected graphs of fixed order and size with maximal index: Some spectral bounds, *Linear Algebra and Appl.*, (432)9(2010), 2361-2372.
9. F. Belardo, E.M. Li Marzi, S.K. Simić, J.F. Wang, On the index of necklaces, *Graphs and Combinatorics*, 26(2010), 163-172.
10. F. Belardo, E.M. Li Marzi, S.K. Simić, Trees with minimal index and diameter at most four, *Discrete Math.*, 310(2010), 1708-1714.

11. A. Krapež, S.K. Simić, D.V. Tošić, Parastrophically uncancellable quasigroup equations, *Aequat. Math.*, 79(2010), 261-280.
12. F. Belardo, E.M. Li Marzi, S.K. Simić, Combinatorial approach for computing the characteristic polynomial of a matrix, *Linear Algebra Appl.*, (433)8-10(2010), 513-1523.
13. X. Geng, S. Li, S.K. Simić, On the spectral radius of quasi- k -cyclic graphs, *Linear Algebra Appl.*, (433)8-10(2010), 1561-1572.
14. D. Stevanović, Resolution of AutoGraphiX conjectures relating the index and matching number of graphs, *Linear Algebra Appl.* 433 (2010), 1674--1677.
15. M. Aouchiche, P. Hansen, D. Stevanović, A sharp upper bound on algebraic connectivity using domination number, *Linear Algebra Appl.* 432 (2010), 2879--2893.

Chemical graph theory

1. I. Gutman, J. Đurđević, Cycles in dicyclopenta-derivatives of benzenoid hydrocarbons, *MATCH Communications in Mathematical and in Computer Chemistry* 65 (2011) 785-798.
2. I. Gutman, J. Đurđević, D. Bašić, D. Rašović, On π -electron configuration of cyclopenta-derivatives of benzenoid hydrocarbons, *Indian Journal of Chemistry* 49A (2010) 853-860.
3. I. Gutman, S. Marković, S. Jeremić, A case of breakdown of the Kekulé-structure model, *Polycyclic Aromatic Compounds* 30 (2010) 240-246.
4. S. Marković, J. Đurđević, S. Jeremić, I. Gutman, Diradical character of some fluoranthenes, *Journal of the Serbian Chemical Society* 75 (2010) 1241-1249.
5. S. B. Bozkurt, A. D. Güngör, I. Gutman, Randić spectral radius and Randić energy, *MATCH Communications in Mathematical and in Computer Chemistry* 64 (2010) 321-334.
6. W. Li, X. Li, I. Gutman, Volkmann trees and their molecular structure descriptors, u knjizi: I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors - Theory and Applications II*, Univ. Kragujevac, Kragujevac, 2010, pp. 231-246.
7. M. Ghorbani, M. A. Hosseinzadeh, I. Gutman, The truncated Randić-type indices, *Kragujevac Journal of Science* 32 (2010) 45-56.

8. I. G. Yero, J. A. Rodriguez-Velazquez, I. Gutman, Estimating the higher-order Randić index, *Chemical Physics Letters* 489 (2010) 118-120.
9. I. Gutman, Edge versions of topological indices, u knjizi: I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors - Theory and Applications II*, Univ. Kragujevac, Kragujevac, 2010, pp. 3-20.
10. S. Jeremić, S. Radenković, I. Gutman, Cyclic conjugation in benzo-annelated coronenes, *Macedonian Journal of Chemistry and Chemical Engineering* 29 (2010) 63-69.
11. T. Balaban, J. Đurđević, I. Gutman, S. Jeremić, S. Radenković, Correlations between local aromaticity indices of bipartite conjugated hydrocarbons, *Journal of Physical Chemistry A* 114 (2010) 5870-5877.
12. A. Heydari, I. Gutman, On the terminal Wiener index of thorn graphs, *Kragujevac Journal of Science* 32 (2010) 57-64.
13. I. Gutman, B. Furtula, A survey on terminal Wiener index, u knjizi: I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors - Theory and Applications I*, Univ. Kragujevac, Kragujevac, 2010, pp. 173-190.
14. B. Furtula, I. Gutman, Geometric-arithmetic indices, u knjizi: I. Gutman, B. Furtula (Eds.), *Novel Molecular Structure Descriptors - Theory and Applications I*, Univ. Kragujevac, Kragujevac, 2010, pp. 137-172.
15. D. Vukičević, J. Đurđević, I. Gutman, On the number of Kekulé structures of fluoranthene congeners, *Journal of the Serbian Chemical Society* 75 (2010) 1093-1098.
16. S. Jeremić, S. Radenković, I. Gutman, Cyclic conjugation in benzo-annelated triphenylenes, *Journal of the Serbian Chemical Society* 75 (2010) 943-950.
17. I. Gutman, S. Radenković, W. Linert, Pairwise energy effect of cyclic conjugation in benzo-annelated perylenes, *Monatshefte für Chemie* 141 (2010) 401-407.
18. S. B. Bozkurt, A. D. Güngör, I. Gutman, A. S. Cevik, Randić matrix and Randić energy, *MATCH Communications in Mathematical and in Computer Chemistry* 64 (2010) 239-250.
19. I. Gutman, Theory of the PCP effect and related phenomena, *Journal of Mathematical Chemistry* 47 (2010) 1309-1312.

20. S. Stanković, S. Marković, I. Gutman, S. Sretenović, Hydrogen-mediated Stone-Wales isomerization of dicyclopenta[de,mn]anthracene, *Journal of Molecular Modeling* 16 (2010) 1519-1527.
21. M. Mateljević, V. Božin, I. Gutman, Energy of a polynomial and the Coulson integral formula, *Journal of Mathematical Chemistry* 48 (2010) 1062-1068.
22. S. Li, X. Li, H. Ma, I. Gutman, On triregular graphs whose energy exceeds the number of vertices, *MATCH Communications in Mathematical and in Computer Chemistry* 64 (2010) 201-216.
23. A. Ilić, M. Bašić, I. Gutman, Triply equienergetic graphs, *MATCH - Communications in Mathematical and in Computer Chemistry* 64 (2010) 189-200.
24. I. Gutman, M. Robbiano, E. Andrade Martins, D. M. Cardoso, L. Medina, O. Rojo, Energy of line graphs, *Linear Algebra and Its Applications* 433 (2010) 1312-1323.
25. T. Balaban, T. K. Dickens, I. Gutman, R. B. Mallion, Ring currents and the PCP rule, *Croatica Chemica Acta* 83 (2010) 209-215.
26. H. Bamdad, F. Ashraf, I. Gutman, Lower bounds for Estrada index and Laplacian Estrada index, *Applied Mathematics Letters* 23 (2010) 739-742.
27. O. Khormali, A. Iranmanesh, I. Gutman, A. Ahmadi, Generalized Schultz index and its edge versions, *MATCH Communications in Mathematical and in Computer Chemistry* 64 (2010) 783-798.
28. M. Robbiano, E. Andrade Martins, I. Gutman, Extending a theorem by Fiedler and applications to graph energy, *MATCH Communications in Mathematical and in Computer Chemistry* 64 (2010) 145-156.
29. B. Furtula, I. Gutman, S. Jeremić, S. Radenković, Effect of a ring on cyclic conjugation in another ring: Applications to acenaphthylene-type polycyclic conjugated molecules, *Journal of the Serbian Chemical Society* 75 (2010) 83-90.
30. I. Gutman, Kekulé structures in fluoranthenes, *Zeitschrift für Naturforschung* 65a (2010) 473-476.
31. G. Fath-Tabar, B. Furtula, I. Gutman, A new geometric-arithmetic index, *Journal of Mathematical Chemistry* 47 (2010) 471-486.
32. I. Gutman, K. Salem, A fully benzenoid system has a unique maximum cardinality resonant set, *Acta Applicandae Mathematicae* 112 (2010) 15-19.

33. I. Gutman, B. Zhou, B. Furtula, The Laplacian-energy like invariant is an energy like invariant, *MATCH Communications in Mathematical and in Computer Chemistry* 64 (2010) 85-96.
34. K. C. Das, I. Gutman, Estimating the vertex PI index, *Zeitschrift für Naturforschung* 65a (2010) 430-434.
35. S. Majstorović, I. Gutman, A. Klobučar, Tricyclic biregular graphs whose energy exceeds the number of vertices, *Mathematical Communications* 15 (2010) 213-222.
36. I. Gutman, On a class of integrals encountered in theoretical chemistry, *International Journal of Chemical Modeling* 2 (2010) 335-341.
37. I. Gutman, W. Xiao, Distance in trees and Laplacian matrix, *International Journal of Chemical Modeling* 2 (2010) 327-334.
38. K. C. Das, I. Gutman, Estimating the Wiener index by means of number of vertices, number of edges, and diameter, *MATCH Communications in Mathematical and in Computer Chemistry* 64 (2010) 647-660.
39. W. So, M. Robbiano, N. M. M. de Abreu, I. Gutman, Applications of a theorem by Ky Fan in the theory of graph energy, *Linear Algebra and Its Applications* 432 (2010) 2163-2169.
40. S. Wagner, I. Gutman, Maxima and minima of the Hosoya index and the Merrifield-Simmons index: A survey of results and techniques, *Acta Applicandae Mathematicae* 112 (2010) 323-346.
41. B. Furtula, A. Graovac, D. Vukičević, Augmented Zagreb index, *J. Math. Chem.*, 48(2)(2010), 370–380.
42. D. Stevanović, Counterexamples to conjectures on graphs with greatest edge-Szeged index, *MATCH Commun. Math. Comput. Chem.* 64 (2010), 603—606
43. D. Stevanović, A. Ilić, Distance spectral radius of trees with fixed maximum degree, *Electron. J. Linear Algebra* 20 (2010), 168--179.
44. D. Stevanović, Approximate energy of dendrimers, *MATCH Commun. Math. Comput. Chem.* 64 (2010), 65--73.
45. P.W. Fowler, D. Stevanović, M. Milošević, Counterexamples to a conjecture of Dias on eigenvalues of chemical graphs, *MATCH Commun. Math. Comput. Chem.* 63 (2010), 727--736.
46. A. Ilić, S. Klavžar, D. Stevanović, Calculating the degree distance of partial Hamming graphs, *MATCH Commun. Math. Comput. Chem.* 63 (2010), 411--424.

47. A. Ilić, A. Ilić, D. Stevanović, On the Wiener index and Laplacian coefficients of graphs with given diameter or radius, *MATCH Commun. Math. Comput. Chem.* 63 (2010), 91--100.
48. A. Ilić, D. Stevanović, The Estrada index of chemical trees, *J. Math. Chem.* 47 (2010), 305--314

Graph spectra in computer science

1. D. Cvetković, T. Davidović, A. Ilić, S.K. Simić, Graphs for small multiprocessor interconnected networks, *Applied Math. Computation*, 217(2010), 2468-2480.
2. D. Cvetković, S.K. Simić, Graph spectra in computer science, *Linear Algebra Appl.*, to appear, DOI: 10.1016/j.laa.2010.11035

Structural graph theory

1. N. Trotignon, K. Vušković, A structure theorem for graphs with no cycle with unique chord and its consequences, *Journal of Graph Theory* 63 (1) (2010), 31-67.
2. R.C.S. Machado, C.M.H. de Figueiredo, K. Vušković, Chromatic index of graphs with no cycle with unique chord, *Theoretical Computer Science* 411 (2010), 1221-1234.
3. K. Vušković, Even-hole-free graphs: a survey, *Applicable Analysis and Discrete Mathematics* 4 (2010), 219-240.

Optimization

1. A. Savić, J. Kratica, M. Milanović, Đ. Dugošija, "A mixed integer linear programming formulation of the maximum betweenness problem", *European Journal of Operational Research*, Vol. 206, No. 3, pp. 522-527, 2010.
2. O. Babić, M. Kalić, G. Pavković, S. Dožić, M. Čangalović, Heuristic approach to the airline schedule disturbances problem, *Transportation Planning and Technology* 33, No. 3, 2010, 257-280
3. M. Bouchard, M. Čangalović, A. Hertz, On a reduction of the interval coloring problem to a series of bandwidth coloring problems, *Journal of Scheduling* 13, No. 6, 2010, 583-595

4. Lj. Pavlović, Comment on "Complete solution to a conjecture on Randić index" , European Journal of Operational Research, 207 (2010), 539-542.
5. P. Stanojević, M. Marić, J. Kratica, N. Bojović, M. Milenković, "Mathematical optimization for the train timetabling problem", *Mathematica Balkanica (NewSeries)*, Vol. 24, pp. 303-312, 2010.

PROCEEDING PAPERS

1. V. Kovačević Vujčić, M. Čangalović, N. Mladenović, J. Kratica, Determining the metric dimension of hypercubes by a variable neighborhood search, *Zbornik radova, XXXVII Simpozijum o operacionim istraživanjima, SYM-OP-IS 2010*, septembar 21-24, 2010, Tara, str. 397-399
2. T. Davidović, D. Ramljak, M. Šelmić, D. Teodorović, Parallel Bee Colony Optimization for Scheduling Independent Tasks on Identical Machines, *Proc. 37th Symp. on Operational Research, SYM-OP-IS 2010*, pp. 389-392, Tara, Sept. 21-24, 2010.
3. G. Singh, A. Ernst, T. Davidović, Variable Neighborhood Search for Resource-Constrained Scheduling, *Proc. 37th Symp. on Operational Research, SYM-OP-IS 2010*, pp. 417-420, Tara, Sept. 21-24, 2010.
4. D. Teodorović, T. Davidović, M. Šelmić, M., D. Ramljak, An Application of a Meta-heuristic Algorithm to p -center Location Problem (in Serbian), *Proc. Symp. on information technology, YUINFO 2010*, (on CD 026.pdf), Kopaonik, March 03-06, 2010.

PAPERS IN PRINT

3. J.F. Wang, S.K. Simić, Q.X. Huang, F. Belardo, E.M. Li Marzi, Laplacian spectral characterization of disjoint union of paths and cycles, *Linear Multilinear Algebra*, to appear, doi: 10.1080/03081081003605777.
4. F. Belardo, E.M. Li Marzi, S.K. Simić, J.F. Wang, Graphs whose (signless) Laplacian spectral radius does not exceed the Laplacian Hoffman limit value, to appear.
5. F. Belardo, E.M. V. de Filippo, S.K. Simić, Computing the permanent polynomial of a matrix from a combinatorial viewpoint, *MATCH*, to appear.

6. M. Anđelić, C. Fonseca, S.K. Simić, D.V. Tošić, Some further bounds for the Q-index of nested split graphs, *Journal Math. Sciences*, to appear.
7. T. Biyikoglu, S.K. Simić, Z. Stanić, Some notes on cographs, *Ars Combinatoria*, to appear.
8. N. Otero, S. Fias, S. Radenković, P. Bultinck, A. M. Graña, M. Mandado, How does aromaticity rule the thermodynamic stability of hydroporphyrines?, *Chem.-Eur. J. to appear*.
9. J. Kratica, M. Milanović, Z. Stanimirović, D. Tošić, "An evolutionary based approach for solving a capacitated hub location problem", *Applied Soft Computing*, DOI: 10.1016/j.asoc.2010.05.035
10. J. Kratica, A. Savić, V. Filipović, M. Milanović, "Solving the task assignment problem with a variable neighborhood search", *Serdica Journal of Computing*, to appear.
11. P. Ren, T. Aleksić, D. Emms, R. Wilson, E. Hancock, Quantum walks, Ihara zeta functions and cospectrality in regular graphs, *Quantum Information Processing* DOI: 10.1007/s11128-010-0205-y.
12. P. Ren, T. Aleksić, R. Wilson, E. Hancock, A Polynomial Characterization of Hypergraphs Using the Ihara Zeta Function, *Pattern Recognition Journal*, DOI:10.1016/j.patcog.2010.06.011
13. P. Ren, E. Hancock, R. Wilson, T. Aleksić, Ihara Coefficients: A Flexible Tool for Higher Order Learning, accepted for conference S+SSPR 2010, Cesme, Izmir, Turkey, August 18-21, 2010.