

**PROJECT 174033:
GRAPH THEORY AND MATHEMATICAL PROGRAMMING
WITH APPLICATIONS TO CHEMISTRY AND COMPUTER
SCIENCE**

Publications in 2011

MONOGRAPHS AND CHAPTERS IN MONOGRAPHS

D. Cvetković, I. Gutman (Eds.), *Selected Topics on Applications of Graph Spectra*, Collection of Papers Vol. 14 (22), Mathematical Institute of the Serbian Academy of Sciences and Arts, Belgrade, 2011.

D. Stevanović, Applications of graph spectra in quantum physics, in: *Selected topics on applications of graph spectra* (D. Cvetković, I. Gutman, eds.), Collection of Papers Vol. 14 (22), Mathematical Institute of the Serbian Academy of Sciences and Arts, Belgrade, 2011, pp. 85-112.

I. Gutman, Hyperenergetic and hypoenergetic graphs, , in: *Selected topics on applications of graph spectra* (D. Cvetković, I. Gutman, eds.), Collection of Papers Vol. 14 (22), Mathematical Institute of the Serbian Academy of Sciences and Arts, Belgrade, 2011, pp. 113-135.

I. Gutman, B. Borovićanin, Nullity of graphs: An updated survey, , in: *Selected topics on applications of graph spectra* (D. Cvetković, I. Gutman, eds.), Collection of Papers Vol. 14 (22), Mathematical Institute of the Serbian Academy of Sciences and Arts, Belgrade, 2011, pp. 137-154.

I. Gutman, H. Deng, S. Radenković, The Estrada index: An updated survey, , in: *Selected topics on applications of graph spectra* (D. Cvetković, I. Gutman, eds.), Collection of Papers Vol. 14 (22), Mathematical Institute of the Serbian Academy of Sciences and Arts, Belgrade, 2011, pp. 155-174.

Z. Stanimirović, J. Kratica, V. Filipović, D. Tošić, *Evolutional approach to solving hub location problems*, (Serbian), Zavod za udžbenike i nastavna sredstva, 2011, ISBN: 978-86-17-17501-4.

M. V. Diudea, C. L. Nagy, A. Ilić, Diamond D5 - a Novel Class of Carbon Allotropes, in: *Carbon Bonding and Structures*, Ed. M. V. Putz, Springer, 2011, pp. 273-291.

DOCTORAL DISSERTATIONS

Aleksandar Ilić, *Extremal problems and algorithms for graph invariants based on eigenvalues and distances*, (Serbian), doctoral thesis, University of Niš, Faculty of Science, March 2011. Supervisor Dragan Stevanović.

Milica Andjelić, *Spectral results related with the structure of graphs*, doctoral thesis, University of Aveiro, Portugal, July 2011. Supervisors Domingos Cardoso and Slobodan Simić.

Jelena Đurđević, *Contribution to the knowledge of cyclic conjugation in derivatives of acenaphthylenes and fluoranthenes*, (Serbian), doctoral thesis, University of Kragujevac, Faculty of Science, December 2011, Supervisor Ivan Gutman.

JOURNAL PAPERS

Subproject 1: Spectral graph theory

Z. Huang, H. Deng, S.K. Simić, On the spectral radius of cactuses with perfect matchings, *Appl. Anal. Discrete Math.* 5(2011), 14-21.

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*, 59(5)(2011), 531-539.

F. Belardo, E.M. V. de Filippo, S.K. Simić, Computing the permanental polynomial of a matrix from a combinatorial viewpoint, *MATCH Commun. Math. Comput. Chem.* 66(2011), 381-396.

T. Bıyıkoglu, S.K. Simić, Z. Stanić, Some notes on cographs, *Ars Combin.*, 100(2011), 421-434.

M. Andjelić, C.M. da Fonseca, S.K. Simić, D.V. Tošić, On bounds for the index of double nested graphs, *Linear Algebra Appl.*, 435(2011), 2475-2490.

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, *Linear Algebra Appl.*, 435(2011), 2913-2920.

M. Petrović, T. Aleksić, S.K. Simić, Further results on the least eigenvalue of connected graphs, *Linear Algebra Appl.*, 435(2011), 2303-2313.

S. Li, S.K. Simić, D.V. Tošić, Q. Zhao, On ordering bicyclic graphs with respect to the Laplacian spectral radius, *Applied Math. Lett.*, 24(12)(2011), 2186-2192.

M. Anđelić, C.M. da Fonseca, Sufficient conditions for positive definiteness of tridiagonal matrices revisited, *Positivity* 15(2011), 155-159.

M. Anđelić, C.M. da Fonseca, R.Mamede, On the number of P-vertices of some graphs, *Linear Algebra Appl.* 434(2)(2011), 514-525.

Petrović M., Aleksić T., Simić V., On the least eigenvalue of cacti, *Linear Algebra Appl.*, 435(10)(2011), 2357-2364.

M. Rašajski, Z. Radosavljević, B. Mihailović, Maximal reflexive cacti with four cycles: The approach via Smith graphs, *Linear Algebra and Its Applications* 435(2011), 2530-2543.

M. Petrović, Z. Radosavljević, M. Rašajski, Cacti with a Given Spectral Property, *Scientific Publications of the State University of Novi Pazar, Ser. A: Appl. Math. Inform. And Mech.* 3(2)(2011), 101-115.

D. Stevanović, Two spectral characterizations of regular, bipartite graphs with five eigenvalues, *Linear Algebra Appl.* 435(2011), 2612-2625.

I. Jovanović, Z. Stanić, Spectral distances of graphs, *Linear Algebra Appl.*, (2011), doi: 10.1016/j.laa.2011.08.019.

M. Bašić, A. Ilić, On the automorphism group of integral circulant graphs, *Electr. J. Comb.* 18(2011), #P68

M. Lepović, The conjugate main eigenvalues of vertex deleted subgraphs of a strongly regular graphs, *New Zealand Journal of Mathematics*, 40(2010), 67-74.

Subproject 2: Chemical graph theory

K. C. Das, I. Gutman, B. Furtula, On the first geometric-arithmetic index of graphs, *Discrete Applied Mathematics* 159(2011), 2030-2037.

I. Gutman, J. Y. Shao, The energy change of weighted graphs, *Linear Algebra and Its Applications* 435(2011), 2425-2431.

N. Abreu, D. M. Cardoso, I. Gutman, E. A. Martins, M. Robbiano, Bounds for the signless Laplacian energy, *Linear Algebra and Its Applications* 435(2011), 2365-2374.

Z. Yarahmadi, A. R. Ashrafi, I. Gutman, First and second extremal bipartite graphs with respect to PI index, *Mathematical and Computer Modelling* 54(2011), 2460-2463.

- I. Gutman, B. Furtula, Estimating the second and third geometric-arithmetic indices, *Hacettepe Journal of Mathematics and Statistics* 40(2011), 69-76.
- S. K. Ayyaswamy, S. Balachandran, I. Gutman, Upper bound for the energy of strongly connected digraphs, *Applicable Analysis and Discrete Mathematics* 5(2011), 37-45.
- I. Gutman, G. V. Milovanović, Calculating a class of integrals encountered in theoretical chemistry, *Bulletin de l'Académie Serbe des Sciences et des Arts (Classe des Sciences Mathématiques et Naturelles)* 143(2011), 1-19.
- K. C. Das, I. Gutman, D. Vukičević, One-two descriptor of graphs, *Bulletin de l'Académie Serbe des Sciences et des Arts (Classe des Sciences Mathématiques et Naturelles)* 143(2011), 37-47.
- A. Alwardi, N. D. Soner, I. Gutman, On the common--neighborhood energy of a graph, *Bulletin de l'Académie Serbe des Sciences et des Arts (Classe des Sciences Mathématiques et Naturelles)*, 143(2011), 49-59.
- I. Gutman, Multiplicative Zagreb indices of trees, *Bulletin of Society of Mathematicians Banja Luka* 18(2011), 17-23.
- I. Gutman, Multiplicative Zagreb indices of trees, *Bulletin of International Mathematical Virtual Institute* 1(2011), 13-19.
- H. Khodashenas, M. J. Nadjafi-Arani, A. R. Ashrafi, I. Gutman, A new proof of the Szeged-Wiener theorem and a new characterization of block graphs, *Kragujevac Journal of Mathematics* 35(2011), 165-172.
- I. Gutman, A. R. Ashrafi, G. H. Fath-Tabar, Graph ham energy [Equienergetic graphs], *Farhang va Andishe-e-Riazi [Culture and Thinking of Mathematics]* 15(1389), 41-50 [in Persian, 1389 ~ 2011].
- K. C. Das, I. Gutman, B. Furtula, Survey on geometric-arithmetic indices of graphs, *MATCH Communications in Mathematical and in Computer Chemistry* 65(2011), 595-644.
- B. Horoldagva, I. Gutman, On some vertex-degree-based graph invariants, *MATCH Communications in Mathematical and in Computer Chemistry* 65(2011), 723-730.
- A. Ilić, I. Gutman, Eccentric connectivity index of chemical trees, *MATCH Communications in Mathematical and in Computer Chemistry* 65(2011), 731-744.
- K. C. Das, F. M. Bhatti, S. G. Lee, I. Gutman, Spectral properties of the He matrix of hexagonal systems, *MATCH Communications in Mathematical and in Computer Chemistry* 65(2011), 753-774.

- I. Gutman, J. Đurđević, Cycles in dicyclopenta-derivatives of benzenoid hydrocarbons, *MATCH Communications in Mathematical and in Computer Chemistry* 65(2011), 785-798.
- T. Došlić, B. Furtula, A. Graovac, I. Gutman, S. Moradi, Z. Yarahmadi, On vertex-degree-based molecular structure descriptors, *MATCH Communications in Mathematical and in Computer Chemistry* 66(2011), 613-626.
- D. Vukičević, I. Gutman, B. Furtula, V. Andova, D. Dimitrov, Some observations on comparing Zagreb indices, *MATCH Communications in Mathematical and in Computer Chemistry* 66(2011), 627-645.
- S. K. Ayyaswamy, S. Balachandran, Y. B. Venkatakrishnan, I. Gutman, Signless Laplacian Estrada index, *MATCH Communications in Mathematical and in Computer Chemistry* 66(2011), 785-794.
- K. Xu, I. Gutman, The greatest Hosoya index of bicyclic graphs with given maximum degree, *MATCH Communications in Mathematical and in Computer Chemistry* 66(2011), 795-824.
- J. Y. Shao, F. Gong, I. Gutman, New approaches for the real and complex integral formulas of the energy of a polynomial, *MATCH Communications in Mathematical and in Computer Chemistry* 66(2011), 849-861.
- B. Furtula, I. Gutman, Relation between second and third geometric-arithmetic indices of trees, *Journal of Chemometrics* 25(2011), 87-91.
- F. M. Brückler, T. Došlić, A. Graovac, I. Gutman, On a class of distance-based molecular structure descriptors, *Chemical Physics Letters* 503(2011), 336-338.
- K. C. Das, I. Gutman, B. Furtula, On atom-bond connectivity index, *Chemical Physics Letters* 511(2011), 452-454.
- A. T. Balaban, I. Gutman, S. Jeremić, J. Đurđević, Effect of benzo-annelation on cyclic conjugation, *Monatshefte für Chemie* 142(2011), 53-57.
- A. T. Balaban, I. Gutman, S. Marković, D. Simijonović, Local aromaticity in benzo- and benzocyclobutadieno-annelated anthracenes, *Monatshefte für Chemie* 142(2011), 797-800.
- S. Marković, J. Đurđević, S. Jeremić, I. Gutman, Triplet fluoranthenes: Aromaticity versus unpaired electrons, *Journal of Molecular Modeling* 17(2011), 805-810.
- A. T. Balaban, I. Gutman, S. Marković, D. Simijonović, J. Đurđević, Local aromaticity in benzo- and benzocyclobutadieno-annelated phenanthrenes, *Polycyclic Aromatic Compounds* 31(2011), 339-349.

- S. Marković, S. Radenković, Z. Marković, I. Gutman, DFT study on singlet diradical character of zethrenes, *Russian Journal of Physical Chemistry A* 85(2011), 2368-2372.
- I. Gutman, Effect of benzocyclobutadieno-annulation on cyclic conjugation, *Indian Journal of Chemistry* 50A(2011), 670-673.
- I. Gutman, B. Furtula, A. T. Balaban, Effect of benzocyclobutadieno-annulation on cyclic conjugation in fluoranthene congeners, *Journal of the Serbian Chemical Society* 76(2011), 733-741.
- I. Gutman, A. T. Balaban, Simple mathematical model for the effect of benzo-annulation on cyclic conjugation, *Journal of the Serbian Chemical Society* 76(2011), 1505-1511.
- X. Xu, F. Wei, I. Gutman, Comparing the energy of two unicyclic molecular graphs, *Kragujevac Journal of Science* 33(2011), 39-44.
- I. Gutman, M. Janošević, S. Radenković, Effect of benzocyclobutadieno-annulation on cyclic conjugation in coronene, *Kragujevac Journal of Science* 33(2011), 45-53.
- D. Stevanović, *Oriented incidence energy and threshold graphs*, *FILOMAT* 25(2)(2011), 1-8.
- D. Stevanović, *Remarks on Fowler-Manolopoulos predictor of fullerene stability*, *MATCH Commun. Math. Comput. Chem.* 66(2011), 285-292
- M. V. Diudea, K. Nagy, C. L. Nagy, A. Ilić, *Omega Polynomial in Puzzle Zeolites*, *MATCH Commun. Math. Comput. Chem.* 65(2011), 143-152.
- M. V. Diudea, A. Ilić, *Omega Polynomial in TiO₂ Crystal Lattices*, *MATCH Commun. Math. Comput. Chem.* 65(2011), 153-162.
- D. Vukičević, J. Đurđević, Bond additive modeling 10. Upper and lower bounds of bond incident degree indices of catacondensed fluoranthenes, *Chemical Physics Letters*, 515(2011), 186-189
- M. V. Diudea, A. Ilić, All pentagonal face multitori, *J. Comput. Theor. Nanosci.* 8(2011), 736-739.
- M. V. Diudea, A. Ilić, K. Varmuza, M. Dehmer, Network Analysis Using a Novel Highly Discriminating Topological Index, *Complexity* (2011), doi:10.1002/cplx.20363
- A. Ilić, M. Bašić, New results on the energy of integral circulant graphs, *Appl. Math. Comp.* 218(2011), 3470-3482.

A. Ilić, B. Zhou, On reformulated Zagreb indices, *Discrete Appl. Math.* (2011), doi:10.1016/j.dam.2011.09.021

A. Ilić, M. Ilić, B. Liu, On the upper bounds for the first Zagreb index, *Kragujevac Journal of Mathematics* 35(2011), 173-182.

N. Otero, S. Fias, S. Radenković, P. Bultinck, A. M. Graña, M. Mandado, How does aromaticity rule the thermodynamic stability of hydroporphyrines? *Chemistry - A European Journal* 17(2011), 3274-3286.

S. Radenković, P. Bultinck, Ring currents in Polycyclic Sodium Clusters, *Journal of Physical Chemistry A* 115(2011), 12493–12502.

S. Radenković, S. Marković, R. Kuč, N. Stanković, The diradical character of polyacenequinododimethides, *Monatshefte für Chemie* 142(2011), 1013-1019.

Subproject 3: Mathematical programming

J. Kratica, M. Milanović, Z. Stanimirović, D. Tošić, An evolutionary based approach for solving a capacitated hub location problem, *Applied Soft Computing*, 11(2011), 1858–1866.

M. Milanović, D. Matić, A. Savić, J. Kratica, Two metaheuristic approaches to solving the p-ary transitive reduction problem, *Appl. Comput. Math.*, 10(2)(2011), 294-308.

T. Davidović, D. Ramljak, M. Šelmić, D. Teodorović, Bee Colony Optimization for the p-Center Problem, *Computers and Operations Research*, 38(10)(2011), 1367--1376.

M. Kuzmanović, V. Kovačević-Vujčić, M. Martić, Three stage entry game: The strategic effect of advertising, *Yugoslav Journal of Operations Research*, 21(2)(2011).

Subproject 4: Structural graph theory and algorithms

N. Trotignon, K. Vušković, On Roussel and Rubio type lemmas and their consequences, *Discrete Mathematics* 311(2011), 684-687.

N. Trotignon, K. Vušković, Combinatorial optimization with 2-joins, *Journal of Combinatorial Theory B* (2011) doi:10.1016/j.jctb.2011.06.002.

A. Ilić, D. Stevanović, L. Feng, G. Yu, P. Dankelmann, Degree distance of unicyclic and bicyclic graphs, *Discrete Appl. Math.* 159(2011), 779-788.

G. Yu, L. Feng, A. Ilić, On the eccentric distance sum of trees and unicyclic graphs, *J. Math. Anal. Appl.* 375(2011), 934-944.

A. Ilić, G. Yu, L. Feng, On the eccentric distance sum of graphs, *J. Math. Anal. Appl.* 381(2011), 590-600.

M. Bouchar, M. Čangalović, A. Hertz, On a reduction of the interval coloring problem to a series of bandwidth coloring problems, *Journal of Scheduling* 13(6)(2010), 583-595.

Subproject 5: Graph spectra in computer science

1. Cvetković D., Simić S.K., Graph spectra in computer science, *Linear Algebra Appl.*, 434(2011), 1545-1562.

2. Cvetković D., Rowlinson P., Stanić Z., Yoon M.-G., Controllable graphs, *Bull. Acad. Serbe Sci. Arts, Cl. Sci. Math. Natur., Sci. Math.* 143(36)(2011), 81-88.

3. Cvetković D., Rowlinson P., Stanić Z., Yoon M.-G., Controllable graphs with least eigenvalue at least -2, *Applicable Analysis and Discrete Mathematics*, 5(2)(2011), 165-175.

P. Van Mieghem, D. Stevanović, F. Kuipers, C. Li, R. van de Bovenkamp, D. Lu and H. Wang, *Decreasing the spectral radius of a graph by link removals*, *Phys. Rev. E* 84(2011), 016101.

P. Ren, T. Aleksić, D. Emms, R. Wilson, E. Hancock, Quantum walks, Ihara zeta functions and cospectrality in regular graphs, *Quantum Information Processing* 10(3)(2011), 405-417.

Papers in the conference proceedings

M. Čangalović, J. Kratica, V. Kovačević-Vujčić, M. Stojanović, Minimal doubly resolving sets of some generalized Petersen graphs, *Proc. 1st International Symposium & 10th Balkan Conference on Operational Research (BALCOR 2011)*, pp. 178-184, 22 - 24 September 2011, Thessaloniki, Greece.

A. Savić, J. Fijuljanin, J. Kratica, Hybrid genetic algorithm for solving of maximum betweenness problem, *Proc. 1st International Symposium & 10th Balkan Conference on Operational Research (BALCOR 2011)*, pp. 402-408, 22 - 24 September 2011, Thessaloniki, Greece.

T. Davidović, D. Ramljak, M. Šelmić, D. Teodorović, MPI Parallelization of Bee Colony Optimization, *Proc. 1st Int. Symp and 10th Balkan Conf. on Operational Research, BALCOR 2011*, Vol. 2, pp. 193-200, Thessaloniki, Greece, Sept. 22-24, 2011.

M. Bruglieri, T. Davidović, S. Roksandić, Optimization of trips to the university: a new algorithm for a carpooling service based on the Variable Neighborhood Search, *Proc. REACT 2011 Shaping Climate Friendly Transport in Europe: Key Findings and Future Directions*, pp. 191-199, Belgrade, Serbia, May 16--17, 2011.

S. Roksandić, D. Urošević, N. Mladenović, T. Davidović, E. Carrizosa, E., Huff Location Model of the Bicycle Parking Services, *Proc. REACT 2011 Shaping Climate Friendly Transport in Europe: Key Findings and Future Directions*, pp. 270-275, Belgrade, Serbia, May 16--17, 2011.

T. Davidović, J. Lazić, V. Maraš, Combinatorial Formulation Guided Local Search for Inland Waterway Routing and Scheduling, *Proc. 13th IASTED International Conference on Control and Applications (on CD 729-091.pdf)*, pp. 241-248, DOI: 10.2316/P.2011.729-091, Vancouver, BC, Canada, June 1-3, 2011.

M. Rašajski, L-graphs, a class of maximal reflexive cacti with three cycles, *Proc. XXXVIII Symposium on Operational Research, SYMOPIS 20011*, pp. 250-253, Zlatibor, Oct. 4-7, 2011.

M. Rašajski, Z. Radosavljević, B. Mihailović, σ -extensions in some classes of maximal reflexive cacti, *Proc. XXXVIII Symposium on Operational Research, SYMOPIS 20011*, pp. 254-257, Zlatibor, Oct. 4-7, 2011.

Papers in press

M. Anđelić, C.M. da Fonseca, S.K. Simić, D.V. Tošić, Connected graphs of fixed order and size with maximal Q-index: Some spectral bounds, *Discrete Appl. Math.*, accepted, doi:10.1016/j.dam.2011.11.001

M. Andjelić, C.M. da Fonseca, S.K. Simić, D.V. Tošić, Some further bounds for the Q-index of nested split graphs, *Journal Math. Sciences*, to appear.

I. Sciriha, S.K. Simić, A note on eigenspaces of some compound graphs, *Quaderni di Matematica della Seconda Università di Napoli*, to appear.

D. Cvetković, S.K. Simić, Spectral graph theory in computer science, *IPSI Transactions Journals*, to appear.

D. Vukičević, J. Đurđević, I. Gutman, Limitations of Pauling Bond Order Concept, *Polycyclic Aromatic Compounds*, in press

M. Radovanović, K. Vušković, A class of three-colorable triangle-free graphs, *Journal of Graph Theory*, accepted.

J. Kratica, T. Kostić, D. Tošić, Đ. Dugošija, V. Filipović, A genetic algorithm for the routing and carrier selection problem, *Computer Science and Information Systems – COMSIS*, accepted for publication.

J. Kratica, D. Tošić, V. Filipović, Đ. Dugošija, A new genetic representation for quadratic assignment problem, *Yugoslav Journal of Operations Research*, accepted for publication

J. Kratica, V. Kovačević-Vujčić, M. Čangalović, M. Stojanović, Minimal doubly resolving sets and the strong metric dimension of Hamming graphs, *Applicable Analysis and Discrete Mathematics*, accepted for publication, doi: 10.2298/AADM111116023K

Other papers

A. Ilić, S. Klavžar, Y. Rho, Generalized Fibonacci cubes, *Discrete Math.* (2011), doi:10.1016/j.disc.2011.02.015

S. Stanimirović, P. Stanimirović, A. Ilić, Ballot matrix as Catalan matrix power and related identities, *Discrete Appl. Math.* (2011), doi:10.1016/j.dam.2011.10.016

A. Ilić, A. Ilić, On the number of restricted Dyck paths, *Filomat* 25(2011), 191-201.

Lj. S. Velimirović, S. R. Rančić, M. Lj. Zlatanović, Rigidity and flexibility analysis of a kind of surfaces of revolution and visualization, *Applied Mathematics and Computation*, 217(2011), 4612-4619.

T. Aleksić, I. Gutman, Review of the book: *P. Van Mieghem: Graph Spectra for Complex Networks*, *MATCH Communications in Mathematical and in Computer Chemistry* 67(2012), 557-558.