

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

Publications in 2012

MONOGRAPHS AND CHAPTERS IN MONOGRAPHS

1. X. Li, Y. Shi I. Gutman,
Graph Energy, Springer,
New York, 2012, pp. XI+266.
2. I. Gutman, Y. Zhang, M. Dehmer, A. Ilić,
Altenburg, Wiener, and Hosoya polynomials,
in: I. Gutman, B. Furtula (Eds.), *Distance in Molecular Graphs - Theory*, University of
Kragujevac, Kragujevac, 2012, pp. 49–70.

DOCTORAL DISSERTATIONS

1. Tatjana Aleksić,
Grafovi čija je najmanja karakteristična vrednost minimalna u nekim klasama grafova,
(Graphs whose least eigenvalue is minimal in some classes of graphs, Serbian), doctoral
thesis, University of Kragujevac, Faculty of Science, September 2012, Supervisor
Miroslav Petrović

JOURNAL PAPERS

Subproject 1: Spectral graph theory

1. M. Andelić, C.M.da Fonseca,S.K. Simić, and D.V. Tošić,
Some further bounds for the Q-index of nested split graphs,
J. Math. Sci. (N. Y.) **182** (2012), no. 2, 193-198.
2. M. Andelić, C.M.da Fonseca,S.K. Simić, and D.V. Tošić,
Connected graphs of fixed order and size with maximal Q-index: some spectral bounds,
Discrete Appl. Math. **160** (2012), no. 4-5, 448-459.
3. M. Andelić, C.M.da Fonseca, T. Koledin, Z. Stanić,
Sharp spectral inequalities for connected bipartite graphs with maximal Q-index,

Ars Math. Contemp. **6** (2013), no. 1, 171-185.

4. M. Andelić, T. Koledin, Z. Stanić,

Nested graphs with bounded second largest (signless) Laplacian eigenvalue,
Electronic Journal of Linear Algebra, **24**(2012), 181-201.

5. I. Jovanović, Z. Stanić,

Spectral distances of graphs,

Linear Algebra and its Applications, **436**(2012), 1425-1435.

6. Z. Stanić,

Some graphs whose second largest eigenvalue does not exceed $\sqrt{2}$,

Linear Algebra and its Applications, **437**(2012), 1812-1820.

7. M. Milatović, Z. Stanić,

The nested split graphs whose second largest eigenvalue is equal to 1,

Novi Sad Journal of Mathematics, **42**(2012), 33-42.

8. I. Gutman, B. Furtula, E. O. D. Andriantiana, M. Cvetić,

More trees with large energy and small size,

MATCH Commun. Math. Comput. Chem. **68** (2012) 697–702.

9. T. Tamizh Chelvam, S. Raja, I. Gutman,

Strongly regular integral circulant graphs and their energies,

Bulletin of International Mathematical Virtual Institute **2** (2012) 9–16.

10. I. Gutman,

Comparative studies of graph energies,

Bulletin de l'Academie Serbe des Sciences et des Arts (Classe des Sciences Mathématiques et Naturelles) **144** (2012) 1–17.

11. I. Gutman,

Bounds for all graph energies,

Chemical Physics Letters **528** (2012) 72–74.

12. G.H. Fath-Tabar, A.R. Ashrafi, D. Stevanović,

Spectral Properties of Fullerenes,

J. Comput. Theor. Nanos. **9** (2012), 327–329.

13. D. Stevanović, M. Petković, M. Bašić,

On the Diameter of Integral Circulant Graphs,

Ars Combinatoria **106** (2012), 495–500.

14. M. Lepović,

On strongly regular graphs with $m_2 = qm_3$ and $m_3 = qm_2$,

Serdica Math. J. **37**(2011), 353-364.

15. B. Liu, Lj. Pavlović, J. Liu, T. Divnić, M. Stojanović,
On the conjecture of Aouchiche and Hansen about the Randić index,
Discrete Mathematics, **313**(3) (2013), 225–235.

Subproject 2: Chemical graph theory

1. K. C. Das, K. Xu, I. Gutman,
Comparison between Kirchhoff index and the Laplacian–energy–like invariant,
Linear Algebra and Its Applications **436** (2012) 3661–3671.
2. H. Abdo, D. Dimitrov, I. Gutman,
On the Zagreb indices equality,
Discrete Applied Mathematics **160** (2012) 1–8.
3. I. Gutman, S. Wagner,
The matching energy of a graph,
Discrete Applied Mathematics **160** (2012) 2177–2187.
4. M. Ghorbani, M. Songhori, I. Gutman,
Modified Narumi–Katayama index,
Kragujevac Journal of Science **34** (2012) 57–64.
5. I. Gutman, M. Ghorbani,
Some properties of the Narumi–Katayama index,
Applied Mathematics Letters **25** (2012) 1435–1438.
6. J. Liu, I. Gutman, Z. Mu, Y. Zhang,
 q -Wiener index of some compound trees,
Applied Mathematics and Computation **218** (2012) 9528–9535.
7. B. Furtula, I. Gutman, M. Ivanović, D. Vukičević,
Computer search for trees with minimal ABC index,
Applied Mathematics and Computation **219** (2012) 767–772.
8. M. Eliasi, A. Iranmanesh, I. Gutman,
Multiplicative versions of first Zagreb index,
MATCH Commun. Math. Comput. Chem. **67**, (2012) 217–230.
9. Y. Zhang, I. Gutman, J. Liu, Z. Mu,
 q -Analog of Wiener index,
MATCH Commun. Math. Comput. Chem. **67**, (2012) 347–356.
10. I. Gutman, B. Furtula, M. Ivanović,
Notes on trees with minimal atom–bond connectivity index,

MATCH Commun. Math. Comput. Chem. **67**, (2012) 467–482.

11. R. Cruz, I. Gutman, J. Rada,
Convex hexagonal systems and their topological indices,
MATCH Commun. Math. Comput. Chem. **68**, (2012) 97–108.
12. I. Gutman, B. Furtula,
Trees with smallest atom–bond connectivity index,
MATCH Commun. Math. Comput. Chem. **68** (2012) 131–136.
13. K. C. Das I. Gutman, B. Horoldagva,
Comparing Zagreb indices and coindices of trees,
MATCH Commun. Math. Comput. Chem. **68**, (2012) 189–198.
14. Y. Zhang, Z. Zhang, W. Chen, I. Gutman, Y. Li,
Predicting nucleosome positions by using the dinucleotide compositions of the Nucleosomes,
MATCH Commun. Math. Comput. Chem. **68** (2012) 633–644.
15. K. C. Das, I. Gutman, B. Furtula,
On atom–bond connectivity index,
Filomat **26** (2012) 733–738.
16. I. Gutman, L. Feng, G. Yu,
On the degree resistance distance of unicyclic graphs,
Transactions on Combinatorics **1**(2) (2012) 27–40.
17. T. Réti, I. Gutman,
Relations between ordinary and multiplicative Zagreb indices,
Bulletin of International Mathematical Virtual Institute **2** (2012) 133–140.
18. B. Arsić, I. Gutman, K. C. Das, K. Xu,
Relations between Kirchhoff index and Laplacian–energy–like invariant
Bulletin de l'Académie Serbe des Sciences et des Arts (Classe des Sciences Mathématiques et Naturelles) **144** (2012) 59–70.
19. H. S. Ramane, A. B. Ganagi, I. Gutman,
On a conjecture on the diameter of line graphs of graphs of diameter two,
Kragujevac Journal of Mathematics **36** (2012) 59–62.
20. K. P. Narayankar, S. B. Lokesh, V. Mathad, I. Gutman,
Hosoya polynomial of Hanoi graphs,
Kragujevac Journal of Mathematics **36** (2012) 77–83.
21. C. Adiga, A. Bayad, I. Gutman, A. S. Shrikanth,
The minimum covering energy of a graph,

22. I. Gutman,
Estimating the Laplacian–energy–like molecular structure descriptor,
Zeitschrift für Naturforschung **67a** (2012) 403–406.
23. D. Vukičević, J. Đurđević, I. Gutman,
Limitations of Pauling bond order concept,
Polycyclic Aromatic Compounds **32** (2012) 36–47.
24. Z. Zhang, Y. Zhang, I. Gutman,
Predicting nucleosome position in yeast: Using the absolute frequency,
Journal of Biomolecular Structure and Dynamics **29** (2012) 1081–1088.
25. I. Gutman, J. Tošović, S. Radenković, S. Marković,
On atom–bond connectivity index and its chemical applicability,
Indian Journal of Chemistry **51A** (2012) 690–694.
26. J. Đurđević, I. Gutman,
Phenyl-cyclopentadienyl rule,
Macedonian Journal of Chemistry and Chemical Engineering **31** (2012) 1–15.
27. M. Marković, J. Đurđević, I. Gutman,
Cyclic conjugation in benzo– and benzocyclobutadieno–annelated terrylenes and higher
rylenes,
Journal of the Serbian Chemical Society **77** (2012) 751–759.
28. I. Gutman, B. Furtula,
Vertex-degree–based molecular structure descriptors of benzenoid systems and
Phenylenes,
Journal of the Serbian Chemical Society **77** (2012) 1031–1036.
29. Z. Du, A. Ilić,
On AGX conjectures regarding average eccentricity,
MATCH Commun. Math. Comput. Chem. **69** (2013) 579–587.
30. S. Radenković, S. Marković, V. Milenković,
Electronic structure study of the triplet azulene-like molecules,
Chemical Physics Letters **545** (2012) 132–137.
31. S. Radenković, J. Đurđević, P. Bultick,
Local aromaticity of the five-membered rings in acenaphthylene derivates,
Physical Chemistry Chemical Physics **14** (2012) 14067–14078.
32. S. Radenković, I. Gutman, P. Bultinck,
Comparative study of aromaticity in tetraoxa[8]circulenes,

Journal of Physical Chemistry A **116** (2012) 9421-9430.

33. D. Deb, S. Duley, S. Radenković, P. Bultinck, P. K. Chattaraj, M. Bhattacharjee, Heterotrimetallic compounds containing Mo-M-Li [M = K, Rb and Cs] clusters: synthesis, structure, bonding, aromaticity and theoretical investigations of Li_2M_2 [M = K and Rb] and Cs_4 Rings, *Physical Chemistry Chemical Physics*, **14** (2012) 15579-15592.
34. I. Gutman, J. Đurđević, S. Radenković, Z. Matović, Anomalous cyclic conjugation in the perylene/bisanthrene homologous series, *Monatshefte für Chemie*, **143** (2012) 1649-1653.
35. S. Radenković, P. Bultinck, I. Gutman, J. Đurđević, On induced current density in the perylene/bisanthrene homologous series, *Chemical Physics Letters*, **552** (2012) 151-155.
36. M. Dehmer, M. Grabner, B. Furtula, Structural discrimination of networks by using distance, degree and eigenvalue-based measures, *PloS ONE* **7** (7) (2012) e38564.
37. H. Shabani, A. R. Ashrafi, I. Gutman, B. Furtula, On extensions of Wiener index, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 589-596.
38. M. Milošević, T. Reti, D. Stevanović, On the Constant Difference of Zagreb Indices, *MATCH Commun. Math. Comput. Chem.* **68** (2012), 157–168.
39. D. Stevanović, M. Milanič, Improved Inequality between Zagreb Indices of Trees, *MATCH Commun. Math. Comput. Chem.* **68** (2012), 147–156.
40. Ž. Vukićević-Kovijanić, D. Stevanović, Bicyclic graphs with extremal values of PI index, *Discrete Appl. Math.* **161** (2013), 395-403.
41. A. Ilić, B. Zhou, On reformulated Zagreb indices, *Discrete Appl. Math.* **160** (2012), 204-209.
42. A. Ilić, G. Yu, L. Feng, Harary index of trees, *Utilitas Math.* **87** (2012) 21-31.
43. M. Dehmer, A. Ilić,

Location of zeros of Wiener and Distance Polynomial,
PLoS ONE **7** (2012), e28328.

Subproject 3: Mathematical programming

1. J. Kratica, V. Kovačević-Vujčić, M. Čangalović, M. Stojanović,
Minimal doubly resolving sets and the strong metric dimension of some convex polytopes,
Applied Mathematics and Computation, **218**(19), (2012), 9790–9801.
2. N. Mladenović, J. Kratica, V. Kovačević-Vujčić, M. Čangalović,
Variable neighborhood search for metric dimension and minimal doubly resolving set problems,
European Journal of Operational Research, **220** (2012), 328–337.
3. 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, **6**(1), (2012), 63–71.
4. 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, **9**(1), (2012), 49-62.
5. J. Kratica,
An electromagnetism-like approach for solving the low autocorrelation binary sequence problem,
International Journal of Computers, Communications & Control, **7**(4), (2012), 687-694.
6. T. Davidović, M. Šelmić, D. Teodorović, D. Ramljak,
Bee Colony Optimization for Scheduling Independent Tasks to Identical Processors,
Journal of Heuristics, **18**(4), (2012) , 549-569.
7. N. Mladenović, D. Urošević, S. Hanafi, A. Ilić,
A general variable neighborhood search for the one-commodity pickup-and-delivery travelling salesman problem,
Eur. J. Oper. Research **220** (2012), 270-285.
8. J. Kratica, M. Leitner, I. Ljubić,
Variable neighborhood search for solving the balanced location problem,
Electronic Notes in Discrete Mathematics, **39**, (2012), 21-28.
9. N. Mladenović, J. Kratica, V. Kovačević-Vujčić, M. Čangalović,
Variable neighborhood search for the strong metric dimension problem,
Electronic Notes in Discrete Mathematics, **39**, (2012), 51-57.

10. D. Matić, J. Kratica, V. Filipović, Đ. Dugošija,
Variable neighborhood search for multiple level warehouse layout problem,
Electronic Notes in Discrete Mathematics, **39** (2012), 161-168.

11. T. Davidović, T. G. Crainic,
MPI Parallelization of Variable Neighborhood Search,
Electronic Notes in Discrete Mathematics, **39** (2012), 241-248.

12. T. Divnić, Lj. Pavlović,
A Slight Modification of the First Phase of the Simplex Algorithm,
Yugoslav Journal of Operational Research, **22**(1) (2012), 107-114.

Subproject 4: Structural graph theory and algorithms

1. N. Trotignon and K. Vušković,
Combinatorial optimization with 2-joins,
Journal of Combinatorial Theory B **102**(1) (2012) 153-185.

2. P. Charbit, M. Habib, N. Trotignon and K. Vušković,
Detecting 2-joins faster,
Journal of Discrete Algorithms, **17**, (2012), 60-66.

3. P. Aboulker, M. Radovanović, N. Trotignon and K. Vušković,
Graphs that do not contain a cycle with a node that has at least two neighbors on it,
SIAM Journal on Discrete Mathematics, **26**(4) (2012), 1510-1531.

4. D. Stevanović,
Comparing the Zagreb indices of the NEPS of graphs,
Appl. Math. Comput. **219** (2012), 1082-1086.

5. S. Stanimirović, P. Stanimirović, A. Ilić,
Ballot matrix as Catalan matrix power and related identities,
Discrete Appl. Math. **160** (2012) 344-351.

6. A. Ilić, S. Klavžar, Y. Rho,
Generalized Fibonacci cubes,
Discrete Math. **312** (2012), 2-11.

7. A. Ilić, S. Klavžar, Y. Rho,
Generalized Lucas cubes,
Appl. Anal. Discrete Math. **6** (2012) 82-94.

8. A. Ilić, S. Klavžar, Y. Rho,

The index of a binary word,
Theoret. Comput. Sci. **452** (2012) 100-106.

9. A. Ilić, S. Klavžar, Y. Rho,
Parity index of binary words and powers of prime words,
Electron. J. Combin. **19** (2012) #P44.

10. A. Ilić,
On the extremal properties of the average eccentricity,
Comp. Math. Appl. **64** (2012), 2877-2885.

Subproject 5: Graph spectra in computer science

1. D. Cvetković, S. K. Simić,
Spectral graph theory in computer science,
The IPSI BgD Transactions on Advanced Research, **8**(2012), No. 2, 35-42.

2. B. Arsić, D. Cvetković, S. K. Simić, M. Škarić,
Graph spectral techniques in computer sciences,
Applicable Analysis and Discrete Mathematics, **6**(2012), No. 1, 1-30.

3. D. Cvetković,
Complexity indices for the travelling salesman problem and data mining,
Transactions of Combinatorics, **1**(2012), No. 1, 35-43.

4. D. Cvetković,
Spectral recognition of graphs,
Yugoslav Journal of Operations Research, **22**(2012), No.2, 145-161.

Papers in conference proceedings

1. V. Maraš, R. Konings, Z. Radmilović, T. Davidović,
Routing feeder container ships with empty container repositioning,
Proc. MARITIME TRANSPORT V - Technological, Innovation and Research,
Barcelona, June 27-29, 2012, 232-252.

2. M. Bruglieri, A. Colorni, T. Davidović, S. Roksandić,
A Matheuristic Approach for the University Carpooling Problem,
Proc. CTW 2012 - 11th Cologne-Twente Workshop on Graphs and Combinatorial Optimization,
Munchen, Germany, May 29-31, 2012, 46-50.

3. S. Kordić, B. Dragović, T. Davidović, N. Kovač,
 A Combinatorial Algorithm for Berth Allocation Problem in Container Port,
Proc. International Association of Maritime Economists Conference, IAME 2012
 Taipei, Sept. 6-8, 2012.
4. T. Davidović, J. Lazić, N. Mladenović, S. Kordić, N. Kovač, B. Dragović, B.,
 MIP-Heuristics for Minimum Cost Berth Allocation Problem,
Proc. International Conference on Traffic and Transport Engineering, ICTTE 2012
 Belgrade, Nov. 29-30, 2012, 21-28.
5. M. Rašajski, Z. Radosavljević, B. Mihailović,
 Modifications of Smith trees in some classes of maximal reflexive cacti,
*Proc. International conference on pure and applied combinatorics and its connections
 with Geometry, Graph Theory and Algebra, Combinatorics* 2012,
 Perugia, Italy, Sept. 10-15, 2012.
6. B. Mihailović, M. Rašajski,
 Bounds for the second largest eigenvalue of a connected graph with a cut-vertex,
*Proc. International conference on pure and applied combinatorics and its connections
 with Geometry, Graph Theory and Algebra, Combinatorics* 2012,
 Perugia, Italy, Sept. 10-15, 2012.
7. V. Filipović, J. Kratica, A. Savić, Đ. Dugošija,
 The modification of genetic algorithms for solving the balanced location problem,
Proc. 5th Balkan Conference in Informatics,
 Novi Sad, Serbia, 16-20 September 2012, pp. 243-246.
8. R. Jovanović, M. Dražić, V. Tošić, M. Stanojević, M. Čangalović,
 Self-financing modulation of air navigation charges to incentivise a more efficient use of
 airspace capacity,
Proc. 5th International Conference on Research in Air Transportation ICRAT 2012,
 University of California, Berkeley, 2012, electronic version (www.icrat.org/icrat/)
9. M. Rašajski, Z. Radosavljević, B. Mihailović,
 Modifikacije Smitovih stabala u strukturi nekih klasa maksimalnih refleksivnih grafova,
Proc. XXXIX Symp. on Operational Res. SYMOPIS 2012,
 Tara, Sept. 25-28, 2012, 221-224.
10. I. Jovanović,
 Network Alignment Algorithms,
Proc. XXXIX Symp. on Operational Res. SYMOPIS 2012,
 Tara, Sept. 25-28, 2012,
11. J. Kratica, V. Kovačević-Vujčić, M. Čangalović,
 An electromagnetism-like method for the strong metric dimension problem,

Zbornik radova XXXIX Simpozijuma iz operacionih istraživanja SYM-OP-IS 2012,
Tara, 2012, 351-354.

Papers in press

1. Davidović, T., Jakšić, T., Ramljak, D., Šelmić, M., Teodorović, D.,
MPI Parallelization Strategies for Bee Colony Optimization,
OPTIMIZATION, Special Issue entitled "Advances in Discrete Optimization",
dedicated to BALCOR 2011.
DOI:10.1080/02331934.2012.749258
2. T. G. Crainic, T. Davidović, D. Ramljak,
DESIGNING PARALLEL META-HEURISTIC METHODS,
In *High Performance and Cloud Computing in Science and Education*, Despotović-Zrakić, M., Milutinović, V., Belić, A., (eds.) 2012. (Accepted),
CIRRELT Research Report [CIRRELT-2012-28](#).
3. D. Stevanović, M. Milošević, P. Hic, M. Pokorný,
Proof of a conjecture on distance energy of complete multipartite graphs,
accepted for publication in *MATCH Commun. Math. Comput. Chem.*
4. L. Feng, G. Yu, A. Ilić, D. Stevanović,
The signless Laplacian spectral radius of graphs on surfaces,
Linear Multilinear Algebra (2012), DOI: 10.1080/03081087.2012.696249
5. M.V.G. da Silva and K. Vušković,
Decomposition of Even-hole-free graphs with star cutsets and 2-joins,
to appear in *Journal of Combinatorial Theory B*. DOI: 10.1016/j.jctb.2012.10.001
6. M. Radovanović and K. Vušković,
A class of three-colorable triangle-free graphs,
to appear in *Journal of Graph Theory*. DOI:10.1002/jgt.21651
7. M. Andelić, C.M.da Fonseca, A. Erić,
Nonsingular acyclic matrices with full number of P-vertices,
to appear in *Linear Multilinear Algebra*.
8. M. Andelić, D.M. Cardoso, S.K. Simić,
Relations between (k,t)-regular sets and star complements,
to appear in *Czechoslovak Math. J.*
9. T. Koledin, Z. Stanić,
Regular bipartite graphs with three distinct non-negative eigenvalues,
to appear in *Linear Algebra and its Applications*

10. L. Feng, W. Liu, A. Ilić, G. Yu,
Degree distance of unicyclic graphs with given matching number,
 to appear in *Graphs Comb.*, (2012), DOI: 10.1007/s00373-012-1143-5
11. A. Ilić,
 Note on the harmonic index of a graph,
 to appear in *ARS Comb.* (2012)
12. A. Ilić, M. Ilić,
 Generalizations of Wiener polarity index and Terminal Wiener index,
 to appear in *Graphs Comb.* (2012), DOI: 10.1007/s00373-012-1215-6
13. A. Ilić, N. Milosavljević,
 The weighted vertex PI index,
 to appear in *Math. Comp. Model.* (2012), DOI 10.1016/j.mcm.2012.08.001
14. I. Gutman, J. Djurdjević, Z. Matović, M. Marković,
 Verifying the modes of cyclic conjugation in tetrabenzo[bc,ef,op,rs]circumanthracene, to
Journal of the Serbian Chemical Society, in press.
15. J. Kratica,
 A mixed integer quadratic programming model for the low autocorrelation binary
 sequence problem,
Serdica Journal of Computing, Accepted for publication
16. J. Kratica,
 An electromagnetism-like method for the maximum set splitting problem,
Yugoslav Journal of Operations Research, Vol. 22, No. 2, 2012., in press
 DOI:10.2298/YJOR110704010K
17. I. Gutman, B. Furtula, M. B. Ahmadi, S. A. Hosseini, P. S. Nowbandegani, M.
 Zarrinderakht,
 The ABC index conundrum,
FILOMAT, accepted.
18. I. Sciriha, S.K. Simić,
 A note on eigenspaces of some compound graphs,
Quaderni di Matematica della Seconda Università di Napoli, to appear.
19. T. Divnić, Lj. Pavlović,
 Proof of the first part of the conjecture of Aouchiche and Hansen about the Randić index,
Discrete Applied Mathematics (2012), doi: 10.1016/j.dam.2012.11.004 .