Dr Svetlana Marković, full professor
CURRICULUM VITAE

BASIC INFORMATION

Name:	Svetlana Marković
Maiden name:	Petrović
Date and place of birth:	April 18, 1959, Kruševac, Serbia
Address:	Faculty of Science, 12 Radoja Domanovića, Serbia Tel: ++ (381) 34 335 039 Fax: ++ (381) 34 335 040 e-mail: mark@kg.ac.rs, svetlana.markovic@pmf.kg.ac.rs

EDUCATION

1966 - 1978: Primary and secondary schooling in Kruševac, Serbia

1978 - 1983: Study of chemistry at the University of Kragujevac, Faculty of Science, Serbia
1983: B. Sc. degree in chemistry

1988: M. Sc. degree in chemistry (University of Kragujevac, Faculty of Science)

1992: Ph. D. degree in chemistry (University of Kragujevac, Faculty of Science)
Field of research: Mathematical and computational chemistry

Post-doctoral studies:
1999 – 2001: Technikon Pretoria, Department of Chemistry and Physics
Field of research: Chemistry under supercritical conditions
Lecturing: Physical Chemistry 2

EMPLOYMENT

1986 - 1993: Teaching assistant at the Faculty of Science, Kragujevac
1993 – 2003: Docent at the Faculty of Science, Kragujevac

2003 – 2009: Associate professor at the Faculty of Science, Kragujevac
2009 – present: Full professor at the Faculty of Science, Kragujevac

Lecturing: Computers in chemistry
Programming in chemistry
Introduction to chemoinformatics
Physical chemistry 1
Molecular modeling 1
Molecular modeling 2
Methodology of scientific work in chemistry
Molecular modeling in organic chemistry

Mentorship: Supervisor of many diploma works and two doctoral dissertations:
Dr Igor Đurović, 2015
Dr Jelena Tošović, 2019

SCIENTIFIC AREAS OF RESEARCH

Prof. Svetlana Marković is engaged in scientific research in the field of theoretical physical, computational, and mathematical chemistry. Her early work was devoted to examining the dependence of physicochemical properties of substances on molecular structure using chemical graph theory, as well as computer modeling of these dependencies. Recent work includes the study of various chemical phenomena using *ab initio* and DFT methods, such as mechanisms of chemical reactions (e.g., the Kolbe-Schmitt reactions with phenoxides and naphthoxides of alkali metals, phenylselenoetherification of unsaturated alcohols, Heck reactions, etc.), diradical character of different classes of hydrocarbons, hydrogen bond, spectroscopic properties and mechanisms of antioxidative action of phenolic compounds, etc. She has reviewed a huge number of scientific papers and has won many certificates from reputable publishing houses and journals.

PUBLICATIONS

Prof. Svetlana Marković has published 105 scientific papers, of which 96 in journals from the SCI list, and 6 professional papers. She is the author of one monograph, one chapter in a monograph and two textbooks. She has participated in 42 international and national conferences.

Scientific papers

105. Žiko Milanović, Jelena Tošović, Svetlana Marković, Zoran Marković
Comparison of the scavenging capacities of phloroglucinol and 2,4,6-trihydroxypyridine towards HO• radical: a computational study
RSC Adv. 10 (2020) 43262-43272. DOI: 10.1039/d0ra08377a
ISSN: 2046-2069, M22, IF(2019)= 3,119

104. Izudin Redžepović, Svetlana Marković, Boris Furtula
Dependence of the Enthalpy of Formation of Phenols on Molecular Structure – Semiempirical Study
Polycyc. Arom. Comp. DOI: 10.1080/10406638.2019.1696379
ISSN: 1040-6638, M22, IF(2019)= 1,894

103. Izudin Redžepović, Svetlana Marković
Theoretical study on the heat of formation of some polycyclic aromatic hydrocarbons
Chem. Pap. 74 (2020) 829-836. DOI: 10.1007/s11696-019-00914-7
ISSN: 2585-7290, M23, IF(2018)=1,246

102. Izudin Redžepović, Svetlana Marković, Boris Furtula
On Structural Dependence of Enthalpy of Formation of Catacondensed Benzenoid Hydrocarbons
MATCH Commun. Math. Comput. Chem. 82(3) (2019) 663-678.
ISSN: 0340-6253, M21, IF(2017)=2,580

101. Jelena Tošović, Svetlana Marković
Antioxidative activity of chlorogenic acid relative to trolox in aqueous solution – DFT study
Food Chem. 278 (2019) 469-475. DOI: https://doi.org/10.1016/j.foodchem.2018.11.070
ISSN: 0308-8146, M21a, IF(2019)=6,306

100. Ana Gligorijević, Svetlana Marković, Izudin Redžepović, Boris Furtula
Application of spectral graph theory on the enthalpy change of formation of acyclic saturated ketones
J. Serb. Chem. Soc. 83 (2018) 1339-1349. https://doi.org/10.2298/JSC180906086G
ISSN: 0352-5139, M23, IF(2018)=0,828

99. Jelena Tošović, **Svetlana Marković**
Reactivity of chlorogenic acid towards hydroxyl and methyl peroxy radicals relative to trolox in nonpolar media
Theor. Chem. Acc. **137** (2018) 76. DOI: 10.1007/s00214-018-2251-y.
ISSN: 1432-881X, **M22**, IF(2016)=**1,890**

98. Adrijana Burmudžija, **Svetlana Marković**, Jovana Muškinja, Anka Pejović, Jelena Tošović
Influence of counterion on the methylation of some ambident nucleophiles: DFT study
React. Kinet. Cat. **123** (2018) 201-214. DOI: 10.1007/s11144-017-1263-2.
ISSN: 1878-5190, **M23**, IF(2016)=**1,264**

97. Izudin Redžepović, **Svetlana Marković**, Jelena Tošović
ANTIOXIDATIVE ACTIVITY OF CAFFEIC ACID – MEDHANISTIC DFT DTUDY
Kragujevac J. Sci. **39** (2017) 109-122. DOI: 10.5937/KgJSci1739109R.
ISSN: 1450-9636, UDC: 541.127:547.587.52, **M51**

96. Jelena Tošović, **Svetlana Marković**, Jasmina M. Dimitrić Marković, Miloš Mojović, Dejan Milenković
Antioxidative mechanisms in chlorogenic acid
Food Chem. **237** (2017) 390-398. DOI:
http://dx.doi.org/10.1016/j.foodchem.2017.05.080.
ISSN: 0308-8146, **M21a**, IF(2016)=**4,529**

95. Jelena Tošović, **Svetlana Marković**
Structural and Antioxidative Features of Chlorogenic Acid

Croat. Chem. Acta **89(4)** 535-541 (2016). DOI: http://dx.doi.org/10.5562/cca3026.
ISSN: 0011-1643, **M23**, IF(2016)=**0,586**

94. Jelena Tošović, **Svetlana Marković**, Dejan Milenković, Zoran Marković
Solvation Enthalpies and Gibbs Energies of the Proton and Electron – Influence of Solvation Models
J. Serb. Soc. Comp. Mech. **10(2)** (2016) 66-76. UDC: 539.125.4:66.093.1, 539.124:66.093.1

93. Jelena Tošović, **Svetlana Marković**
Reproduction and interpretation of the UV-vis spectra of some flavonoids
Chem. Pap. **71** (2017) 543-552. DOI: 10.1007/s11696-016-0002-x.
ISSN: 0366-6352, **M22**, IF(2015)=**1,326**

92. Ana Amić, Bono Lučić, Višnja Stepanić, Zoran Marković, **Svetlana Marković**, Jasmina M. Dimitrić Marković, Dragan Amić
Free radical scavenging potency of quercetin catecholic colonic metabolites: Thermodynamics of $2H^+/2e^-$ processes
Food Chem. **218** (2017) 144-151. DOI: 10.1016/j.foodchem.2016.09.018.
ISSN: 0308-8146, **M21a**, IF(2016)=**4,529**

91. **Svetlana Marković**, Jelena Tošović
Comparative study of the antioxidative activities of caffeoylquinic and caffeic acids
Food Chem. **210** (2016) 585-592. DOI: 10.1016/j.foodchem.2016.05.019.

90. **Svetlana Marković**, Jelena Tošović, Jasmina M. Dimitrić Marković
Synergic application of spectroscopic and theoretical methods to the chlorogenic acid structure elucidation
Spectrochim. Acta A **164** (2016) 67-75. DOI: http://dx.doi.org/10.1016/j.saa.2016.03.044.

89. Zoran Marković, Jelena Tošović, Dejan Milenković, **Svetlana Marković**
Revisiting the solvation enthalpies and free energies of the proton and electron in various solvents
Comput. Theor. Chem. **1077** (2016) 11-17. DOI: 10.1016/j.comptc.2015.09.007.

88. **Svetlana Marković**, Jelena Tošović
Application of Time-Dependent Density Functional and Natural Bond Orbital Theories to the UV−vis Absorption Spectra of Some Phenolic Compounds
J. Phys. Chem. A **119** (2015) 9352-9362. DOI: 10.1021/acs.jpca.5b05129.

87. Vladimir P. Petrović, Dušica Simijonović, Slađana B. Novaković, Goran A. Bogdanović, **Svetlana Marković**, Zorica D. Petrović
Structural characterisation of some vanillic Mannich bases: Experimental and theoretical study
J. Mol. Struct. **1098** (2015) 34-40. DOI: 10.1016/j.molstruc.2015.05.040.

86. Vladimir P. Petrović, Dušica Simijonović, Zorica D. Petrović, **Svetlana Marković**
Formation of a vanillic Mannich base – theoretical study
Chem. Pap. **69(9)** (2015) 1244-1252. DOI: 10.1515/chempap-2015-0123.

85. **Svetlana Marković**, Ljubiša Mitrović, Jelena Đurđević, Jelena Tošović, Zorica Petrović
Alkylation of potassium ethyl acetoacetate: HSAB versus Marcus theory
Comput. Theor. Chem. **1066** (2015) 14-19. DOI: 10.1016/j.comptc.2015.05.005.

84. **Svetlana Marković**, Igor Đurović, Zoran Marković
Revisiting the Kolbe–Schmitt reaction of sodium 2-naphthoxide
Theor. Chem. Acc. **134** (2015) 45. DOI: 10.1007/s00214-015-1648-0.

83. Nenad Janković, Zorica Bugarčić, **Svetlana Marković**
Double catalytic effect of $(PhNH_3)_2CuCl_4$ in a novel, highly efficient synthesis of 2-oxo and thioxo-1,2,3,4-tetrahydropyrimidines
J. Serb. Chem. Soc. **80(5)** (2015) 595-604. DOI: 10.2298/JSC141028011J.

82. **Svetlana Marković**, Nenad Janković, Zorica Bugarčić
Influence of the counteranion on the phenylselenoetherification reaction of nerolidol
Monatsh. Chem. **146(2)** (2015) 275-282. DOI: 10.1007/s00706-014-1361-z.

81. Igor Đurović, **Svetlana Marković**, Zoran Marković
Karboksilacija natrijum-2-naftoksida. Preispitivanje mehanizma pomoću meta-hibridnog funkcionala gustine
Carboxylation of sodium 2-naphthoxide. Reinvestigation of the mechanism by means of a hybrid meta density functional theory method
Hem. Ind. **69(5)** (2015) 485-492. DOI:10.2298/HEMIND140625066D.

80. Vladimir P. Petrović, Dušica Simijonović, Marko N. Živanović, Jelena V. Košarić, Zorica D. Petrović, **Svetlana Marković**, Snežana D. Marković
Vanillic Mannich Bases: Synthesis and Screening of Biological Activity. Mechanistic Insight into the Reaction with 4-Chloroaniline
RSC Advances **4** (2014) 24635-24644. DOI: 10.1039/c4ra03909b.

79. Nenad Janković, **Svetlana Marković**, Zorica Bugarčić
DFT study of the mechanism of the phenylselenoetherification reaction of linalool
Monatsh. Chem. **145** (2014) 1287-1296. DOI: 10.1007/s00706-014-1226-5.

78. **Svetlana Marković**, Ivan Gutman, Nataša Simić
Local Aromaticity in Benzo- and Benzocyclobutadieno-annelated Perylenes
J. Serb. Soc. Comp. Mech. **7(1)** (2013) 71-81. UDC: 547.62:544.424.032.1.

77. Violeta Marković, Milan D. Joksović, **Svetlana Marković**, Ivan Jakovljević
Influence of anthraquinone scaffold on E/Z isomer distribution of two thiosemicarbazone derivatives. 2D NMR and DFT studies
J. Mol. Struct. **1058** (2014) 291-297. DOI: 10.1016/j.molstruc.2013.11.025.

76. **Svetlana Marković**, Violeta Marković, Milan D. Joksović, Nina Todorović, Ljubinka Joksović, Vladimir Divjaković, Snežana Trifunović
Debromination of endo-(+)-3-Bromocamphor with Primary Amines
J. Braz. Chem. Soc. **24(7)** (2013) 1099-1108. DOI: 10.5935/0103-5053.20130144.

75. Zoran Marković, Dragan Amić, Dejan Milenković, Jasmina M. Dimitrić-Marković, **Svetlana Marković**
Examination of the chemical behavior of the quercetin radical cation towards some bases
Phys. Chem. Chem. Phys. **15(19)** (2013) 7370-7378. DOI: 10.1039/c3cp44605k.

74. Zoran Marković, Jelena Đorović, Milan Dekić, Milanka Radulović, **Svetlana Marković**
DFT study of free radical scavenging activity of erodiol
Chem. Pap. **67(11)** (2013) 1453-1461. DOI: 10.2478/s11696-013-0402-0.

73. Violeta Marković, **Svetlana Marković**, Ana Janićijević, Marko V. Rodić, Vukadin M. Leovac, Nina Todorović, Snežana Trifunović, Milan D. Joksović

Mechanistic investigation and DFT calculation of the new reaction between S-methylisothiosemicarbazide and methyl acetoacetate
Struct. Chem. **24(6)** (2013) 2127-2136. DOI: 10.1007/s11224-013-0223-3.

72. **Svetlana Marković**, Jelena Đurđević, Milica Vukosavljević, Zorica Petrović
Mechanistic insight into alkylation of the ethyl acetoacetate anion with different ethyl halides
Russ. J. Phys. Chem. A **87(13)** (2013) 2207–2213. DOI: 10.1134/S0036024413130165.

71. Slavko Radenković, **Svetlana Marković**, Vladimir Milenković
Electronic structure study of the triplet azulene-like molecules
Chem. Phys. Lett. **545** (2012) 132-137.

70. Vladimir P. Petrović, **Svetlana Marković**, Zorica D. Petrović
Mechanistic insight into the formation of cinnamates in phosphine-free Heck reaction
Monatsh. Chem. **143** (2012) 1497-1502.

69. Ivan Gutman, Jelena Tošović, Slavko Radenković, **Svetlana Marković**
On atom-bond connectivity index and its chemical applicability
Indian J. Chem. **51A** (2012) 690-694.

68. Zorica D. Petrović, Vladimir P. Petrović, Dušica Simijonović, **Svetlana Marković** *Stereoselective homogeneous catalytic arylation of methyl methacrylate: Experimental and computational study*
J. Mol. Cat. A: Chemical, **356** (2012) 144-151.

67. Slavko Radenković, **Svetlana Marković**, Ratko Kuč, Nevena Stanković
The diradical character of polyacenequinododimethides
Monatsh. Chem., **142** (2011) 1013-1019.

66. Alexandru T. Balaban, Ivan Gutman, **Svetlana Marković,** Dušica Simijonović, Jelena Đurđević
Local aromaticity in benzo- and benzocyclobutadieno-annelated phenanthrenes
Polycyc. Arom. Comp., **31** (2011) 339-349.

65. Zorica D. Petrović, Vladimir P. Petrović, Dušica Simijonović, **Svetlana Marković**
Insight into hydrolytic reaction of N-acetylated L-histidylglycine dipeptide with novel mechlorethamine platinum(II) complex. NMR and DFT study of the hydrolytic reaction
Dalton Trans., **40** (2011) 9284-9288.

64. Zoran S. Marković, **Svetlana Marković**, Jasmina M. Dimitrić-Marković, Dejan Milenković
Structure and Reactivity of Baicalein Radical Cation
Int. J. Quant. Chem., **112(8)** (2012) 2009-2017.

63. Alexandru T. Balaban, Ivan Gutman, **Svetlana Marković,** Dušica Simijonović
Local aromaticity in benzo- and benzocyclobutadieno-annelated anthracenes
Monatsh. Chem. **142** (2011) 797-800.

62. **Svetlana Marković,** Slavko Radenković, Zoran Marković, Ivan Gutman
DFT Study on Singlet Diradical Character of Zethrenes
Russ. J. Phys. Chem. **85(13)** (2011) 2368-2372.

61. Zorica D. Petrović, **Svetlana Marković**, Vladimir P. Petrović, Dušica Simijonović
Triethanolammonium acetate as multifunctional ionic liquid in palladium-catalyzed

green Heck reaction
J. Mol. Mod. **18** (2012) 433-440.

60. Vladimir P. Petrović, **Svetlana Marković**, Zorica D. Petrović
A new aspect of Heck catalyst formation
Monatsh. Chem. **142** (2011) 141-144.

59. **Svetlana Marković**, Jelena Đurđević, Svetlana Jeremić, Ivan Gutman
Triplet fluoranthenes: aromaticity versus unpaired electrons
J. Mol. Mod. **17** (2011) 805-810.

58. **Svetlana Marković**, Milan D. Joksović, Petra Bombicz, Vukadin M. Leovac, Violeta Marković, Ljubinka Joksović
Theoretical study on structural and mechanistic aspects of synthesis of a 3-aminopyrazole derivative
Tetrahedron, **66** (2010) 6205-6211.

57. **Svetlana Marković**, Jelena Đurđević, Svetlana Jeremić, Ivan Gutman
Diradical character of some fluoranthenes
J. Serb. Chem. Soc., **75(9)** (2010) 1241-1249.

56. Ivan Gutman, **Svetlana Marković**, Svetlana Jeremić
A case of breakdown of the Kekulé-structure model
Polycyc. Arom. Comp., **30(4)** (2010) 240-246.

55. Zorica D. Petrović, Dušica Simijonović, Vladimir P. Petrović, **Svetlana Marković**
Diethanolamine and N,N-diethylethanolamine ionic liquids as precatalyst-precursors and reaction media in green Heck reaction protocol
J. Mol. Cat. A, **327(1-2)** (2010) 45-50.

54. Sonja Stanković, **Svetlana Marković**, Ivan Gutman, Silva Sretenović
Hydrogen-mediated Stone-Wales isomerization of dicyclopenta[de,mn]anthracene
J. Mol. Model. **16** (2010) 1519-1527, DOI 10.1007/s00894-010-0669-9.

53. Zorica D. Petrović, Vladimir P. Petrović, Dušica Simijonović, **Svetlana Marković**
Mechanistic Pathways for Oxidative Addition of Aryl Iodides to the Low-Ligated Diethanolamine Palladium(0) Complex in Phosphine-Free Heck Reactions
J. Organomet. Chem. **694(24)** (2009) 3852-3858.

52. Jelena Đurđević, Slavko Radenković, Ivan Gutman, **Svetlana Marković**
Testing the PCP-rule
Monatsh. Chem. **140(11)** (2009) 1305-1309.

51. **Svetlana Marković**, Ana Despotović, Dejan Jovanović, Igor Đurović
Enthalpy of Formation of Acyclic Saturated Ketones
Russ. J. Phys. Chem. **83(9)** (2009) 1430-1435.

50. Sonja Stanković, **Svetlana Marković**, Slavko Radenković, Ivan Gutman
Formation and Isomerization of Dicyclopenta[de,mn]anthracene. Electronic Structure Study
J. Mol. Model. **15(8)** (2009) 953-958.

49. **S. Marković**, Z. D. Petrović, V. Petrović
DFT study on the preactivation reaction of a palladium catalyst precursor in phosphine-free Heck reactions
Monatsh. Chem. **140(2)** (2009) 171-175.

48. **S. Marković**, S. Stanković, S. Radenković, I. Gutman
Thermal isomerization in cyclopenta[fg]aceanthrylene
Monatsh. Chem. **140(2)** (2009) 153-156.

47. **S. Marković**, S. Stanković, S. Radenković, I. Gutman
Electronic Structure Study of Thermal Intraconversions of Some Dicyclopenta-Fused Polycyclic Aromatic Compounds
J. Chem. Inf. Model. **48** (2008) 1984-1989.

46. V. M. Leovac, **S. Marković**, V. Divjaković, K. M. Szécsényi, M. D. Joksović, I. Leban
Structural and DFT studies on molecular structure of Ni(II) chloride complex with pyridoxal semicarbazone (PLSC). Unusual coordination mode of PLSC
Acta Chim. Slov. **55** (2008) 850-860.

45. Z. D. Petrović, **S. Marković**, D. Simijonović, V. Petrović
Mechanistic Insight into Preactivation of a Modern Palladium Catalyst Precursor in Phosphine-free Heck Reactions
Monatsh. Chem. **140(4)** (2009) 371-374.

44. **S. Marković**, I. Đurović, Z. Marković
Formation of Sodium 6-Hydroxy-2-Naphthoate in the Kolbe-Schmitt Reaction
Monatsh. Chem. **139** (2008) 1169-1174.

43. Z. Marković, **S. Marković**
Last Step of the Para Route of the Kolbe-Schmitt Reaction
J. Chem. Inf. Model. **48** (2008) 143-147.

42. Z. Marković, **S. Marković**, I. Đurović
Kolbe-Schmitt Reaction of Sodium 2-Naphthoxide
Monatsh. Chem. **139** (2008) 329-335.

41. Z. Marković, **S. Marković**, N. Manojlović, J. Predojević-Simović
Mechanism of the Kolbe-Schmitt Reaction. Structure of the Intermediate Potassium Phenoxide - CO2 Complex
J. Chem. Inf. Model. **47(4)** (2007) 1520-1525.

40. **S. Marković**, Z. Marković, N. Begović, N. Manojlović
Mechanism of the Kolbe-Schmitt Reaction with Lithium and Sodium Phenoxides
Russ. J. Phys. Chem. **81(9)** (2007) 1392-1397.

39. N. Pejić, S. Blagojević, S. Anić, V. Vukojević, M. Mijatović, J. Ćirić, Z. Marković, **S. Marković**, Lj. Kolar-Anić
Kinetic Determination of Morphine by means of Bray–Liebhafsky Oscillatory Reaction System Using Analyte Pulse Perturbation Technique
Anal. Chim. Acta **582(2)** (2007) 367-374.

38. Zoran Marković, Svetlana Marković, Snežana Zlatanović
Gas Chromatographic Determination of the Degree of Substitution of CMC
Acta Agriculturae Serbica **XII(24)** (2007) 59-68.

37. Z. Marković, **S. Marković**, N. Begović
Influence of Alkali Metal Cations upon the Kolbe-Schmitt Reaction Mechanism
J. Chem. Inf. Model. **46** (2006) 1957-1964.

36. **S. Marković**, Z. Marković, R.I. McCrindle, B.R. Simonović
Kinetics of Extraction of Coal-Tar Pitch Components with Supercritical Carbon Dioxide
Chem. Pap. **61(1)** (2007) 46-50.

35. **S. Marković**

Approximating total π-electron energy of phenylenes in terms of spectral moments

Indian J. Chem. **42A** (2003) 1304-1308.

34. **S. Marković**, Z. Marković, J.P. Engelbrecht, R.I. McCrindle

Spectral moments of polycyclic aromatic hydrocarbons. Solution of a kinetic problem

J. Chem. Inf. Comput. Sci. **42(1)** (2002) 82-86.

33. Z. Marković, J.P. Engelbrecht, **S. Marković**

Theoretical study of the Kolbe-Schmitt reaction mechanism

Z. Naturforsch. **57 a** (2002) 812-818.

32. **S. Marković**, Z. Marković, R.I. McCrindle

Spectral moments of phenylenes

J. Chem. Inf. Comput. Sci. **41(1)** (2001) 112-119.

31. Z. Marković, **S. Marković**, J.P. Engelbrecht, F.D. Visser

Extraction of coal-tar pitch by supercritical carbon dioxide. Dependence of chemical composition of the extracts on temperature, pressure and extraction time

S. Afr. J. Chem. **53(3)** (2000) 179-190.

30. **S. Marković**

Tenth spectral moment for molecular graphs of phenylenes

J. Chem. Inf. Comput. Sci. **39(4)** (1999) 654-658.

29. **S. Marković**, I. Gutman

Spectral moments of the edge adjacency matrix in molecular graphs. Benzenoid hydrocarbons

J. Chem. Inf. Comput. Sci. **39(2)** (1999) 289-293.

28. I. Gutman, **S. Marković**, A. Vesović, E. Estrada

Approximating total π-electron energy in terms of spectral moments. A quantitative approach

J. Serb. Chem. Soc. **63(8)** (1998) 639-646.

27. **S. Marković**, A. Stajković

The evaluation of spectral moments for molecular graphs of phenylenes

Theor. Chem. Acc. **96** (1997) 256-260.

26. I. Gutman, **S. Marković**, Lj. Popović, Z. Spalević, Lj. Pavlović

The relation between the Wiener indices of phenylenes and their hexagonal squeezes

J. Serb. Chem. Soc. **62(3)** (1997) 207-210.

25. I. Gutman, **S. Marković**, A. Stajković, S. Kamidžorac

Correlations between π-electron properties of phenylenes and their hexagonal squeezes

J. Serb. Chem. Soc. **61(10)** (1996) 873-879.

24. **S. Marković**, I. Gutman, J. Šuković

The dependence of the total π-electron energy of isomeric unbranched cata-condensed benzenoid hydrocarbons with a fixed number of bay regions on the number of Kekulé structures

J. Serb. Chem. Soc. **61(7)** (1996) 539-543.

23. **S. Marković**, I. Gutman, Ž. Bančević

Correlation between Wiener and quasi-Wiener indices in benzenoid hydrocarbons

J. Serb. Chem. Soc. **60(7)** (1995) 633-636.

22. I. Gutman, **S. Marković**, D. Vukićević, A. Stajković

The dependence of total π-electron energy of large benzenoid hydrocarbons on the

number of Kekulé structures is non-linear
J. Serb. Chem. Soc. **60(2)** (1995) 93-98.

21. I. Gutman, **S. Marković**, G. G. Hall
Revisiting a simple regularity for benzenoid hydrocarbons. Total π-electron energy versus the number of Kekulé structures
Chem. Phys. Letters **234** (1995) 21-24.

20. I. Gutman, A. Stajković, **S. Marković**, P. Petković
Dependence of total π-electron energy of phenylenes on Kekulé structure count
J. Serb. Chem. Soc. **59(6)** (1994) 367-373.

19. I. Gutman, **S. Marković**
Benzenoid graph with equal maximum eigenvalues
J. Math. Chem. **13** (1993) 213-215.

18. D. Babić, I. Gutman, **S. Marković**, M. Stanković
On the almost-isospectrality concept for benzenoid systems
Commun. Math. Chem. (Match) **28** (1992) 3-12.

17. I. Gutman, **S. Marković**
Almost-isospectral benzenoid systems
Chem. Phys. Letters **185(5-6)** (1991) 473-477.

16. I. Gutman, **S. Marković**, V. Grbović
The smallest pair of isospectral benzenoid systems
J. Serb. Chem. Soc. **56(8-9)** (1991) 553-554.

15. **S. Marković**
Proof of an equality for benzenoid systems
Coll. Sci. Papers Kragujevac **12** (1991) 127-138.

14. **S. Marković**
The evaluation of the eighth moment for benzenoid graphs
Theor. Chim. Acta **81** (1992) 237-244.

13. I. Gutman, G. G. Hall, **S. Marković**, Z. Stanković, V. Radivojević
Effect of bay regions on the total π-electron energy of benzenoid hydrocarbons
Polycyc. Arom. Comp. **2** (1992) 275-282.

12. **S. Marković**, I. Gutman
Dependence of spectral moments of benzenoid hydrocarbons on molecular structure
J. Mol. Struct. (Theochem) **235** (1991) 81-87.

11. **S. Marković**, I. Gutman, S. Živković, M. Stanković
Topological properties of benzenoid systems. XLVIIIb. A further empirical study of Hall's and Cioslowski's formulae
Coll. Sci. Papers Kragujevac **10** (1989) 61-70.

10. I. Gutman, **S. Marković**
Topological properties of benzenoid systems. XLVIIIa. An empirical study of two contradictory formulas for total π-electron energy
Commun. Math. Chem. (Match) **25** (1990) 141-149.

9. I. Gutman, A. Graovac, S. Vuković, **S. Marković**
Some more isomer-undistinguishing approximate formulas for the total π-electron energy of benzenoid hydrocarbons
J. Serb. Chem. Soc. **54(4)** (1989) 189-196.

8. I. Gutman, **S. Marković**, M. Marinković

Investigation of the Cioslowski formula
Commun. Math. Chem. (Match) **22** (1987) 277-284.

7. I. Gutman, **S. Marković**, D. Luković, V. Radivojević, S. Rančić
On Wiener numbers of benzenoid hydrocarbons
Coll. Sci. Papers Kragujevac **8** (1987) 15-34.

6. I. Gutman, Z. Marković, **S. Marković**
A simple method for the approximate calculation of Hosoya's index
Chem. Phys. Letters **134(2)** (1987) 139-142.

5. I. Gutman, **S. Marković**, A. V. Teodorović, Ž. Bugarčić
Isomer-undistinguishing approximate formulas for the total π-electron energy of benzenoid hydrocarbons
J. Serb. Chem. Soc. **51(3)** (1986) 145-149.

4. I. Gutman, **S. Petrović**
On total π-electron energy of benzenoid hydrocarbons
Chem. Phys. Letters **97(3)** (1983) 292-294.

3. I. Gutman, **S. Petrović**, B. Mohar
Topological properties of benzenoid systems. XXA. Matching polynomials and topological resonance energies of peri-condensed benzenoid hydrocarbons
Coll. Sci. Papers Kragujevac **4** (1983) 189-225.

2. I. Gutman, **S. Petrović**, B. Mohar
Topological properties of benzenoid systems. XX. Matching polynomials and topological resonance energies of cata-condensed benzenoid hydrocarbons
Coll. Sci. Papers Kragujevac **3** (1982) 43-90.

1. I. Gutman, **S. Petrović**
Topological properties of benzenoid systems. VII. Approximate formulas for resonance energy
Bull. Soc. Chim. Beograd **46(9)** (1981) 459-464.

Professional papers

6. Светлана Марковић, Слађана Ђорђевић, Изудин Реџеповић, Жико Милановић
Симулирање хемијских спектара помоћу софтвера за молекулско моделирање ПО
Хем. преглед 60(4) (2019) 90-95.

5. Жико Милановић, Јелена Тошовић, Светлана Марковић
Тест за процену укупне антиоксидативне активности заснован на квантно механичким прорачунима – QM-ORSA протокол
Хем. преглед 60(2) (2019) 32-36.

4. Dejan Milenković, Jelena Tošović, Svetlana Marković, Zoran Marković
Reakcije prelaza elektrona: Markusova teorija
Hem. pregled 57(4) (2016) 92-97.

3. Z. Marković, S. Marković, R.I. McCrindle
Određivanje stepena supstitucije karboksimetil celuloze pomoću gasne hromatografije
Nauka Tehnika Bezbednost 1 (2005) 45-53.

2. Z. Marković, S. Marković
Mehanizam Kolbe-Šmitove reakcije - od otkrića do danas

Hem. pregled 43(4) (2002) 84-87.

1. I. Gutman, S. Marković
Benzenoidni ugljovodonici
Hem. pregled 32 (1991) 55-63.

Scientific communications

42. Izudin Redžepović, Svetlana Marković, Boris Furtula
Graph theory based model for the enthalpy of formation of benzenoid hydrocarbons
8th International Conference on Computational Bioengineering, Belgrade, Serbia, September 4-6, 2019, T.4.6, ICCB. ISBN: 978-86-81037-75-1

41. Ana Gligorijević, Svetlana Marković, Izudin Redžepović, Boris Furtula
Dependence of ΔH_f of ketones on structural properties - computational modeling
Sixth Conference of Young Chemists of Serbia, Belgrade, 27th October 2018, TH06 PE 5. ISBN 978-86-7132-072-6.

40. Jelena Tošović, Svetlana Marković (poster)
REACTIVITY OF CHLOROGENIC ACID TOWARD HYDROXYL RADICAL RELATIVE TO TROLOX IN BENZENE
14th International Conference on Fundamental and Applied Aspects of Physical Chemistry, Belgrade, September 24-28, 2018, B-14-P, 125-128.

39. J. Tošović, S. Marković
Behavior of chlorogenic acid dianion towards free radicals in water solution
The 30th International Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences (Math/Chem/Comp, MC^2-30), Dubrovnik, Croatia (2018) p. 18.

38. J. Tošović, S. Marković
Determination of chlorogenic acid structure using combined experimental and theoretical NMR study
AdriaticNMR, Croatia (2018) p. 38. ISBN: 978-953-6076-42-0.

37. Izudin Redžepović, Svetlana Marković, Jelena Tošović
Theoretical investigation of antioxidative activity of caffeic acid
4th South-East European Conference on Computational Mechanics (SEECCM), Kragujevac, July 03-04, 2017, T.2.1., 24.

36. Jelena Tošović, Svetlana Marković, Dejan Milenković
Antioxidative activity of chlorogenic acid: DFT study
The 29th International Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences (Math/Chem/Comp, MC2-29), Dubrovnik, June 19-24, 2017.

35. Svetlana D. Marković, Jelena Đorović, Zorica Petrović, Ana Amić
EXAMINATION OF ANTIOXIDANT ACTIVITY OF THREE DIHYDROXYBENZOIC ACIDS
13th International Conference on Fundamental and Applied Aspects of Physical Chemistry, Belgrade, September 26-30, 2016, B-05-O, 71-74.

34. Svetlana D. Marković, Jelena Tošović
HYDROGEN ATOM TRANSFER MECHANISM IN CHLOROGENIC ACID
13th International Conference on Fundamental and Applied Aspects of Physical

Chemistry, Belgrade, September 26-30, 2016, B-04-O, 67-70.

33. Jelena Tošović, Svetlana Marković, Jasmina M. Dimitrić Marković
STRUCTURAL AND ANTIOXIDATIVE FEATURES OF CHLOROGENIC ACID
Math/Chem/Comp 2016, 28th MC^2 Conference, Dubrovnik, Croatia, June 20-25, 2016.

32. Jelena Tošović, Svetlana Marković, Jasmina M. Dimitrić Marković
Struktura hlorogenske kiseline: spektroskopski i kvantno-mehanički pristup
XXI Savetovanje o biotehnologiji sa međunarodnim učešćem, Čačak, 11.-12. mart 2016, Zbornik radova 21(24) 809-814.

31. Jelena Tošović, Žarko Milošević, Svetlana Marković
Simulation of the UV-Vis Spectra of Flavonoids
15th International Conference on BioInformatics and BioEngineering (BIBE), Belgrade, November 2-4, 2015, T.4.3.2, 66.

30. Jelena Tošović, Svetlana Marković (poster)
Mehanizmi antioksidativne aktivnosti hlorogenske kiseline: termodinamički pristup/ Antioxidative mechanisms of chlorogenic acid: a thermodynamic approach
Treća konferencija mladih hemičara Srbije, Beograd, 24. oktobar 2015, TH P 07, 94.

29. Ana Amić, Bono Lučić, Višnja Stepanić, Zoran Marković, Svetlana Marković, Jasmina Dimitrić Marković, Dragan Amić (poster)
FREE RADICAL SCAVENGING POTENCY OF QUERCETIN AND ITS CATECHOLIC COLONIC METABOLITES: A DFT STUDY
Math/Chem/Comp 2015, 27th MC^2 Conference, Dubrovnik, Croatia, June 12-19, 2015.

28. Svetlana Marković, Igor Đurović, Zoran Marković
CARBOXYLATION OF SODIUM 2-NAPHTHOXIDE. REINVESTIGATION OF THE MECHANISM BY MEANS OF A META-HYBRID FUNCTIONAL
12th International Conference on Fundamental and Applied Aspects of Physical Chemistry, Belgrade, September 22-26, 2014, B-03-O, 120-123.

27. Jelena Đorović, Zoran Marković, Dejan Milenković, Dragan Amić, Svetlana Marković
ANTIOXIDANT ACTIVITY OF QUERCETIN: HAT VERSUS SET-PT MECHANISM
4th International Congress of Serbian Society of Mechanics, Serbia, Vrnjačka Banja 2013, 849-854.

26. Svetlana Marković, Jelena Đurđević, Zorica Petrović (poster)
Mechanism of O- and C-alkylation of ethyl acetoacetate with different ethyl halides
11th International Conference on Fundamental and Applied Aspects of Physical Chemistry, Belgrade, September 24-28, 2012.

25. Svetlana Marković, Slavko Radenković (poster)
Diradicals and singlet diradicals
2nd International Conference on Computation for Science and Technology, Niğde, Turkey, July 9-11, 2012.

24. Z. D. Petrović, V. P. Petrović, S. Marković, D. Simijonović, D. Hadjipavlou-Litina *Classical and non-classical alkylating agent in one. Novel Pt(II) - mechlorethamine complex as artificial metallopeptidase and soybean lipoxygenase inhibitor*
Twelfth Tetrahedron Symposium: Challenges in Organic and Bioorganic Chemistry, Sitges, Spain, 2011.

23. Z. Marković, J. Dimitrić-Marković, S. Marković (poster)

DFT and spectroscopic study of chelation of kaempferol with iron
3rd Quantum Bioinorganic Chemistry Conference, Český Krumlov, Czech Republic, June 25-28, 2011.

22. Vladimir Petrović, Svetlana Marković, Zorica Petrović (poster)
New aspects of the Heck catalyst formation
10th International Conference on Fundamental and Applied Aspects of Physical Chemistry, Belgrade, 2010, 78-80.

21. Svetlana Marković, Slavko Radenković, Zoran Marković, Ivan Gutman (poster)
Diradical character of zethrenes
10th International Conference on Fundamental and Applied Aspects of Physical Chemistry, Belgrade, 2010, 78-80.

20. S. Marković, Z. D. Petrović, V. Petrović, D. Simijonović (poster)
Mechanism of the preactivation process of trans-[$PdCl_2(DEA)_2$] in phosphine-free Heck reactions
9th International Conference on Fundamental and Applied Aspects of Physical Chemistry, Belgrade, 2008.

19. S. Marković, I. Đurović, Z. Marković
Carboxylation reaction of sodium 2-naphthoxide
9th International Conference on Fundamental and Applied Aspects of Physical Chemistry, Belgrade, 2008.

18. S. Marković, A. Despotović, D. Jovanović, I. Đurović (poster)
Dependence of enthalpy of formation of acyclic saturated ketones on molecular structure
9th International Conference on Fundamental and Applied Aspects of Physical Chemistry, Belgrade, 2008.

17. Z. Marković, S. Marković, N. Manojlović, S. Zlatanović
Gasnohromatografsko određivanje stepena supstitucije CMC-a
XI Savetovanje o biotehnologiji, Čačak, 2006.

16. S. Marković, Z. Marković, D. Milenković
Dependence of activation energy of nucleophilic addition of enolate anion of ethyl acetate to ethyl acetate on HOMO-LUMO gap of corresponding reactants
First South-East European Conference on Computational Mechanics, Kragujevac, 2006.

15. Z. Marković, S. Marković, N. Begović (poster)
Mechanism of the Kolbe-Schmitt Reaction with Different Alkali Metal Phenoxides
8th International Conference on Fundamental and Applied Aspects of Physical Chemistry, Belgrade, 2006.

14. S. Marković, D. Milenković, Z. Marković (poster)
Computational investigation of a nucleophilic addition reaction
8th International Conference on Fundamental and Applied Aspects of Physical Chemistry, Belgrade, 2006.

13. Z. Marković, S. Marković
Primena superkritičnih fluida u proizvodnji hrane
Zimska škola za agronome – Zbornik radova, Čačak, 2003.

12. Z. Marković, S. Marković (poster)

Computational analysis of intermediates of the Kolbe-Schmitt reaction
6th International Conference on Fundamental and Applied Aspects of Physical Chemistry, Belgrade, 2002.

11. S. Marković (invited lecture)
Extraction of coal-tar pitch with supercritical carbon dioxide
6th International Conference on Fundamental and Applied Aspects of Physical Chemistry, Belgrade, 2002.

10. Z. Marković, S. Marković, J.P. Engelbrecht, F. D. Visser
Extraction of the coal-tar pitch by supercritical carbon dioxide. Dependence of chemical composition of the extracts on temperature, pressure and extraction time
35th Convention of the South African Chemical Institute, Potchefstroom, RSA, 2000.

9. Z. Marković, J.P. Engelbrecht, S. Marković
Theoretical investigation of the Kolbe-Schmitt reaction mechanism
35th Convention of the South African Chemical Institute, Potchefstroom, RSA, 2000.

8. S. Marković, I. Gutman (poster)
Dependence of the total π-electron energy of benzenoid hydrocarbons on spectral moments
1st International Conference of the Chemical Societies of the South-East European Countries, Halkidiki, Greece, 1998.

7. S. Marković, V. Ivanov-Petrović, I. Gutman (poster)
Primena teorije grafova u hemiji fenilena
Jubilarni naučni skup "Sto godina Srpskog hemijskog društva", Beograd, 1997.

6. S. Marković, I. Gutman
Zavisnost ukupne π-elektronske energije velikih benzenoidnih ugljovodonika od broja Kekuléovih struktura nije linearna
XXXVII Savetovanje Srpskog Hemijskog Društva sa međunarodnim učešćem, Novi Sad, 1995.

5. S. Marković, I. Gutman
Spektralni momenti benzenoidnih ugljovodonika
XXXIII Savetovanje Srpskog Hemijskog Društva, Novi Sad, 1991.

4. I. Gutman, S. Marković
Prilog proučavanju zavisnosti ukupne π-elektronske energije od broja Kekuléovih struktura
XXXI Savetovanje hemičara SR Srbije, Beograd, 1989.

3. I. Gutman, Z. Marković, S. Marković
Jednostavna metoda za računanje Hosoyinog indeksa
XXIX Savetovanje hemičara SR Srbije, Beograd, 1987.

2. Svetlana Petrović, Ivan Gutman (poster)
Approximative formula for the total π-electronic energy
XI jugoslovenski kongres studenata čiste i primenjene hemije sa međunarodnim učešćem, Ljubljana, 1982.
(XI yugoslav congress of students of pure and applied chemistry with international participation)

1. Svetlana Petrović, Ivan Gutman
Simple method for the calculation of the resonance energy of benzenoid hydrocarbons

X jugoslovenski kongres studenata čiste i primenjene hemije sa međunarodnim učešćem, Novi Sad, 1981, 47.
(X yugoslav congress of students of pure and applied chemistry with international participation)