

MIRJANA ECKERT-MAKSIĆ – List of Publications

Scientific Articles

188. M. Eckert-Maksić, I. Antol & M. Vazdar, "Acetamide as the Model of the Peptide Bond: Nonadiabatic Photodynamical Simulations in the Gas Phase and in the Argon Matrix", *Computational and Theoretical Chemistry* **1040** (2014) 136–143.
187. Z. Glasovac & M. Eckert-Maksić, "Effect of Intramolecular Hydrogen Bonds on the Gas-Phase Basicity of Guanidines", *Australian Journal of Chemistry* **67** (2014) 1056–1062.
186. V. Štrukil, E. Lekšić, E. Meštrović & M. Eckert-Maksić, "The Synthesis and Structural Characterization of Peralkylated Triguanide Superbases", *Australian Journal of Chemistry* **67** (2014) 1129–1133.
185. Z. Glasovac, P. Trošelj, I. Jušinski, D. Margetić & M. Eckert-Maksić, "Synthesis of Highly Basic Hexasubstituted Biguanides by Environmentally Friendly Methods", *Synlett* **24** (2013) 2540–2544.
184. Z. Glasovac, F. Pavošević, V. Štrukil, M. Eckert-Maksić, M. Schlangen & R. Kretschmer, "Toward Extension of the Gas-Phase Basicity Scale by Novel Pyridine Containing Guanidines", *International Journal of Mass Spectrometry* **354** (2013) 113–122.
183. V. Štrukil, Z. Glasovac, I. Đilović, D. Matković-Čalogović, L. Šuman, M. Kralj & M. Eckert-Maksić, "Triguanide Derivatives: Synthesis, Crystal Structure and Evaluation of the Proliferation Effect on Some Tumor Cell Lines", *European Journal of Organic Chemistry* (2012) 6785–6797.
182. T. Friščić, I. Halasz, V. Štrukil, M. Eckert-Maksić & R. E. Dinnebier, "Clean and Efficient Synthesis Using Mechanochemistry: Coordination Polymers, Metal–Organic Frameworks and Metallodrugs", *Croatica Chemica Acta* **85** (2012) 367–378.
181. V. Štrukil, M. D. Igrc, M. Eckert-Maksić & T. Friščić, "Click Mechanochemistry: Quantitative Synthesis of "Ready to Use" Chiral Organocatalysts by Efficient Two-Fold Thiourea Coupling to Vicinal Diamines", *Chemistry—a European Journal* **18** (2012) 8464–8473.
180. V. Štrukil, M. D. Igrc, L. Fábíán, M. Eckert-Maksić, S. L. Childs, D. G. Reid, M. J. Duer, I. Halasz, C. Mottillo & T. Friščić, "A Model for a Solvent-Free Synthetic Organic Research Laboratory: Click-Mechanosynthesis and Structural Characterization of Thioureas without Bulk Solvents", *Green Chemistry* **14** (2012) 2462–2473.
179. V. Štrukil, D. Margetić, M. D. Igrc, M. Eckert-Maksić & T. Friščić, "Desymmetrisation of Aromatic Diamines and Synthesis of Non-Symmetrical Thiourea Derivatives by Click-Mechanochemistry", *Chemical Communications* **48** (2012) 9705–9707.
178. I. Antol, M. Eckert-Maksić, M. Vazdar, M. Ruckebauer & H. Lischka, "QM/MM Non-Adiabatic Decay Dynamics of Formamide in Polar and Non-Polar Solvents", *Physical Chemistry Chemical Physics* **14** (2012) 13262–13272.
177. V. Štrukil, I. Đilović, D. Matković-Čalogović, J. Saame, I. Leito, P. Šket, J. Plavec & M. Eckert-Maksić, "Molecular Structure and Acid/Base Properties of 1,2-Dihydro-1,3,5-Triazine Derivatives", *New Journal of Chemistry* **36** (2012) 86–96.
176. S. Faraji, M. Vazdar, V. S. Reddy, M. Eckert-Maksić, H. Lischka & H. Köppel, "Ab Initio Quantum Dynamical Study of the Multi-State Nonadiabatic Photodissociation of Pyrrole", *Journal of Chemical Physics* **135** (2011) 154310.
175. P. Naumov, Y. Topcu, M. Eckert-Maksić, Z. Glasovac, F. Pavošević, M. Kochunnonny & H. Hara, "Photoinduced Rearrangement of Aromatic N-Chloroamides to Chloroaromatic Amides in the Solid State: Inverted $\Pi(N)$ - $\Sigma(N)$ Occupational Stability of Amidyl Radicals", *Journal of Physical Chemistry A* **115** (2011) 7834–7848.
174. I. Škorić, F. Pavošević, M. Vazdar, Ž. Marinić, M. Šindler-Kulyk, M. Eckert-Maksić & D. Margetić, "Thermal Reaction of 3,4-Benzo-8-substituted-3Z,5Z,7E-octatetraenes and Quantum-Chemical Study of the $(8\pi,6\pi)$ -Electrocyclisation", *Organic & Biomolecular Chemistry* **9** (2011) 6771–6778.
173. D. Margetić, I. Zrinski-Antonac, Z. Glasovac, M. Eckert-Maksić & Lj. Maksimović, "Reactions of Dimethyl Carbonate with Aliphatic Amines under High Pressure", *Synthetic Communications* **41** (2011) 2283–2289.
172. D. Schröder, L. Duchácková, I. Jušinski, M. Eckert-Maksić, J. Heyda, L. Tůma & P. Jungwirth, "Characterization of the Triple Ion $(\text{CH}_3)_4\text{N}^+\text{PF}_6^-(\text{CH}_3)_4\text{N}^+$ in the Gas-Phase", *Chemical Physics Letters* **490** (2010) 14–18.
171. D. Margetić, M. Eckert-Maksić, P. Trošelj & Ž. Marinić, "Reaction of 2,5-Bis-Trifluoromethyl-1,3,4-Oxadiazole With 7-Oxanorbornenes Revisited: Experimental and Quantum-Chemical Study of Reaction Stereoselectivity", *Journal of Fluorine Chemistry* **131** (2010) 408–416.
170. Z. Glasovac, V. Štrukil, M. Eckert-Maksić, D. Schröder, M. Schlangen & H. Schwarz, "Coordination Chemistry of Nickel(II) Nitrate With Superbasic Guanidines as Studied by Electrospray Mass Spectrometry", *International Journal of Mass Spectrometry* **290** (2010) 22–31.
169. V. Štrukil, L. Fábíán, D. G. Reid, M. J. Duer, G. J. Jackson, M. Eckert-Maksić & T. Friščić, "Towards an Environmentally-Friendly Laboratory: Dimensionality and Reactivity in the Mechanochemistry of Metal–Organic Compounds", *Chemical Communications* **46** (2010) 9191–9193.
168. M. Eckert-Maksić, M. Vazdar, M. Ruckebauer, M. Barbatti, T. Müller & H. Lischka, "Matrix-Controlled Photofragmentation of Formamide: Dynamics Simulation in Argon by Nonadiabatic QM/MM Method", *Physical Chemistry Chemical Physics* **12** (2010) 12719–12726.

167. M. Eckert-Maksić & I. Antol, "Study of the Mechanism of the N-CO Photodissociation in *N,N*-Dimethylformamide by Direct Trajectory Surface Hopping Simulations", *Journal of Physical Chemistry A* **113** (2009) 12582–12590.
166. M. Eckert-Maksić, H. Lischka, Z. B. Maksić & M. Vazdar, "The Isomerization Barrier in Cyanocyclobutadienes: An *Ab Initio* Multireference Average Quadratic Coupled Cluster Study", *Journal of Physical Chemistry A* **113** (2009) 8351–8358.
165. M. Vazdar, M. Eckert-Maksić, M. Barbatti & H. Lischka, "Excited-state Non-Adiabatic Dynamics Simulations of Pyrrole", *Molecular Physics* **107** (2009) 845–854.
164. Z. Glasovac, M. Eckert-Maksić & Z. B. Maksić, "Basicity of Organic Bases and Superbases in Acetonitrile by the Polarized Continuum Model and DFT Calculations", *New Journal of Chemistry* **33** (2009) 588–597.
163. A. Tintaru, J. Roithová, D. Schröder, L. Charles, I. Jušinski, Z. Glasovac & M. Eckert-Maksić, "Generation and Dissociation Pathways of Singly and Doubly Protonated Bisguanidines in the Gas Phase", *Journal of Physical Chemistry A* **112** (2008) 12097–12103.
162. M. Eckert-Maksić, Z. Glasovac, P. Trošelj, A. Kutt, T. Rodima, I. Koppel & I. A. Koppel, "Basicity of Guanidines with Heteroalkyl Side Chains in Acetonitrile", *European Journal of Organic Chemistry* (2008) 5176–5184.
161. I. Antol, M. Vazdar, M. Barbatti & M. Eckert-Maksić, "The Effect of Protonation on the Photodissociation Processes in Formamide - An *Ab Initio* Surface Hopping Dynamics Study", *Chemical Physics* **349** (2008) 308–318.
160. I. Antol, M. Barbatti, M. Eckert-Maksić & H. Lischka, "Quantum Chemical Calculations of Electronically Excited States: Formamide, its Protonated Form and Alkali Cation Complexes as Case Studies", *Monatshfte fur Chemie* **139** (2008) 319–328.
159. Z. Glasovac, V. Štrukil, M. Eckert-Maksić, D. Schröder, M. Kaczorowska & H. Schwarz, "Gas-phase proton Affinities of Guanidines with Heteroalkyl Side Chains", *International Journal of Mass Spectrometry* **270** (2008) 39–46.
158. I. Antol, M. Eckert-Maksić, M. Ončák, P. Slaviček & H. Lischka, "Photodissociation Pathways of Acetone upon Excitation into the 3s Rydberg State: Adiabatic Versus Diabatic Mechanism", *Collection of Czechoslovak Chemical Communications* **73** (2008) 1475–1494.
157. I. Antol, M. Eckert-Maksić, M. Barbatti & H. Lischka, "Simulation of the Photodeactivation of Formamide in the $n_o-\pi^*$ and $\pi-\pi^*$ states: An *Ab Initio* on-the-fly Surface-Hopping Dynamics Study", *Journal of Chemical Physics* **127** (2007) 234303.
156. M. Barbatti, G. Granucci, M. Persico, M. Ruckebauer, M. Vazdar, M. Eckert-Maksić & H. Lischka, "The on-the-fly Surface-Hopping Program System Newton-X: Application to *Ab Initio* Simulation of the Nonadiabatic Photodynamics of Benchmark Systems", *Journal of Photochemistry and Photobiology a-Chemistry* **190** (2007) 228–240.
155. I. Antol, M. Eckert-Maksić, H. Lischka & Z. B. Maksić, "[2.2.2]Propellane Isomerization by Grob Rearrangement: An *Ab Initio* MR-AQCC study", *European Journal of Organic Chemistry* (2007) 3173–3178.
154. M. Eckert-Maksić & Z. Glasovac, "Computational Study of Deprotonation of Cyclopropane-Fused Quinones", *Polish Journal of Chemistry* **81** (2007) 1109–1121.
153. M. Eckert-Maksić & D. Margetić, "High-Pressure Synthesis of Novel Organometallic Electron Donor-Electron Acceptor Polycyclic Dyads", *High Pressure Research* **27** (2007) 109–114.
152. M. Barbatti, M. Vazdar, A. J. A. Aquino, M. Eckert-Maksić & H. Lischka, "The Nonadiabatic Deactivation Paths of Pyrrole", *Journal of Chemical Physics* **125** (2006) 164323.
151. I. Zrinski, M. Juribašić & M. Eckert-Maksić, "Microwave-Assisted Synthesis of Pyrazoles by 1,3-Dipolar Cycloaddition of Diazo Compounds to Acetylene Derivatives", *Heterocycles* **68** (2006) 1961–1967.
150. M. Eckert-Maksić, M. Vazdar, M. Barbatti, H. Lischka & Z. B. Maksić, "Automerization Reaction of Cyclobutadiene and its Barrier Height: An *Ab Initio* Benchmark Multireference Average-Quadratic Coupled Cluster Study", *Journal of Chemical Physics* **125** (2006) 064310.
149. D. Margetić & M. Eckert-Maksić, "Computational Study on Reactivity of Cyclic Organometallic Dienes Containing Silicon, Germanium and Tin", *New Journal of Chemistry* **30** (2006) 1149–1154.
148. D. Margetić, B. Prugovečki, I. Đilović & M. Eckert-Maksić, "Structure of Diels-Alder Adduct of Phenylated Germole and 1,4-Epoxy-1,4-Dihydronaphthalene Revisited", *Structural Chemistry* **17** (2006) 301–306.
147. D. Margetić, Y. Murata, K. Komatsu & M. Eckert-Maksić, "Synthesis, X-ray, and DFT Study of the Double-Bond Pyramidalization in 1,7,8,9-Tetraphenyl-4,10,10-Trimethyl-4-Aza-10-Silatricyclo[5.2.1.0.2.6]Deca-8-Ene-3,5-Dione and its Germanium Analogue", *Organometallics* **25** (2006) 111–117.
146. Z. Glasovac, B. Kovačević, E. Meštrović & M. Eckert-Maksić, "Synthesis and Properties of Novel Guanidine Bases. *N,N,N'*-tris(3-dimethylaminopropyl)-guanidine", *Tetrahedron Letters* **46** (2005) 8733–8736.
145. M. Eckert-Maksić & Z. Glasovac, "Cycloproparenyl Anions: From Models to Real Systems", *Pure and Applied Chemistry* **77** (2005) 1835–1850.
144. M. Eckert-Maksić, D. Margetić, S. I. Kirin, D. Milić & D. Matković-Čalogović, "High-Pressure Assisted Synthesis of Fused Norbornenes Containing Two 7-Metallonorborene Units", *European Journal of Organic Chemistry* (2005) 4612–4620.
143. M. Eckert-Maksić & Z. Glasovac, "*Ab Initio* Study of the Effect of α -Substituents on the Acidity of Cyclopropabenzene", *Journal of Physical Organic Chemistry* **18** (2005) 763–772.
142. O. Mó, M. Yañez, M. Eckert-Maksić, Z. B. Maksić, I. Alkorta & J. Elguero, "Periodic Trends In Bond Dissociation Energies. A Theoretical Study", *Journal of Physical Chemistry A* **109** (2005) 4359–4365.
141. I. Antol, M. Eckert-Maksić & H. Lischka, "*Ab Initio* MR-CISD Study of Gas-Phase Basicity of Formamide in the First Excited Singlet State", *Journal of Physical Chemistry A* **108** (2004) 10317–10325.
140. I. Antol, M. Eckert-Maksić, H. Lischka & Z. B. Maksić, "On the Bond-Stretch Isomerism in the Benzo[1,2,4,5]Dicyclobutadiene System - An *Ab Initio* MR-AQCC Study", *ChemPhysChem* **5** (2004) 975–981.
139. I. Zrinski, G. Gadanji & M. Eckert-Maksić, "Synthesis, NMR, and Computational Study of 1,2-Diethyl-3-(trimethylsilyl)cyclopropenylum Hexachloroantimonate", *Structural Chemistry* **15** (2004) 195–206.
138. I. Zrinski, N. Novak-Coumbassa & M. Eckert-Maksić, "Novel Organogermanium Compounds via Metalation of 3-Trimethylsilyl-3-ethoxycarbonylcyclopropene Derivatives", *Organometallics* **23** (2004) 2806–2809.
137. I. Alkorta, J. Elguero, M. Eckert-Maksić & Z. B. Maksić, "Influence of the H/F Replacement on the Homoaromaticity of Homotropylium Ion: A GIAO/DFT Theoretical Study", *Tetrahedron* **60** (2004) 2259–2265.
136. I. Antol, Z. Glasovac & M. Eckert-Maksić, "*Ab Initio* MO and DFT Study of Syn-Sesquinorbornatrienyl Dication and its Isoelectronic Boron Analogue", *New Journal of Chemistry* **28** (2004) 880–886.

135. I. Antol, M. Eckert-Maksić & M. Klessinger, "Ab Initio study of Excited State Protonation of Monosubstituted Benzenes", *Journal of Molecular Structure-Theochem* **664** (2003) 309–317.
134. I. Despotović, M. Eckert-Maksić & Z. B. Maksić, D. M. Smith, "In Pursuit of the Elusive Bond-Stretch Isomers by Ab Initio Methods-Benzocyclobutene, Benzo[1,2:4,5] Dicyclobutadiene, and Some Related Substituted Systems", *Journal of Physical Chemistry A* **107** (2003) 10396–10405.
133. M. Eckert-Maksić, Z. Glasovac, H. Maskill & I. Zrinski, "Alkane- and Arenoxodiazonium Ions: Experimental Results Leading to An Ab Initio Theoretical Investigation", *Journal of Physical Organic Chemistry* **16** (2003) 491–497.
132. I. Antol, M. Eckert-Maksić, T. Müller, M. Dallos & H. Lischka, "Valence and Rydberg states of Protonated Formaldehyde", *Chemical Physics Letters* **374** (2003) 587–593.
131. D. Margetić, R. N. Warrener, M. Eckert-Maksić, I. Antol & Z. Glasovac, "A DFT Study of Pyramidalized Alkenes: 7-oxasesquinorbornenes and 7,7'-dioxasesquinorbornenes", *Theoretical Chemistry Accounts* **109** (2003) 182–189.
130. I. Antol, Z. Glasovac, M. C. Hare, M. Eckert-Maksić & S. R. Kass, "On the Acidity of Cyclopropanaphthalenes - Gas Phase and Computational Studies", *International Journal of Mass Spectrometry* **222** (2003) 11–26.
129. I. Zrinski, G. Gadanji & M. Eckert-Maksić, "Lithiation/silylation of Ethyl 2-Alkyl-1-trimethylsilylcycloprop-2-ene-1-carboxylate. Experimental and Computational Study", *New Journal of Chemistry* **27** (2003) 1270–1276.
128. I. Zrinski & M. Eckert-Maksić, "Preparation of Novel Trialkylsilylated Propyne Derivatives From 3-Trimethylsilyl-3-ethoxycarbonylcyclopropene", *Synthetic Communications* **33** (2003) 4071–4077.
127. Z. Glasovac, M. Eckert-Maksić, J. E. Dacres & S. R. Kass, "Gas Phase Formation of 1-Phenylcyclobuten-3-yl and 1-Phenylallyl Anions and a Determination of the Allylic C-H Acidities and Bond Dissociation Energies of 1-Phenylcyclobutene And (E)-1-Phenylpropene", *Journal of the Chemical Society-Perkin Transactions 2* (2002) 410–415.
126. M. Eckert-Maksić, I. Antol, D. Margetić & Z. Glasovac, "syn-Sesquinorbornenyl Carbocations and Their Boron Analogues: An Ab Initio and DFT Study", *Journal of the Chemical Society-Perkin Transactions 2* (2002) 2057–2063.
125. M. Eckert-Maksić, H. Maskill & I. Zrinski, "Acidic and Basic Properties of Nitramide, and the Catalysed Decomposition of Nitramide and Related Compounds: An Ab Initio Theoretical Investigation", *Journal of the Chemical Society-Perkin Transactions 2* (2001) 2147–2154.
124. M. Eckert-Maksić, Z. Glasovac, N. Novak Coumbassa & Z. B. Maksić, "The Mills-Nixon Effect and Chemical Reactivity - Methyl Cation Affinity of Some Cycloalkabenzenes", *Journal of the Chemical Society-Perkin Transactions 2* (2001) 1091–1098.
123. M. Eckert-Maksić, S. Kazazić, S. Kazazić, S. I. Kirin, L. Klasinc, D. Srzić & D. Žigon, "Electron Ionisation Induced Fragmentation of Fused Norbornene Analogues Containing SiMe₂ or GeMe₂ and Oxygen Bridges. Migration of SiMe₂ and GeMe₂ Groups", *Rapid Communications in Mass Spectrometry* **15** (2001) 462–465.
122. Z. Glasovac, M. Eckert-Maksić, K. M. Broadus, M. C. Hare & S. R. Kass, "Benzocyclobutene: The Impact of Fusing a Strained Ring onto Benzene", *Journal of Organic Chemistry* **65** (2000) 1818–1824.
121. M. Eckert-Maksić, V. Rapić, D. Margetić & V. Matonićkin, "Ionic Hydrogenation of 4-Hydroxycoumarin Derivatives", *Heterocyclic Communications* **6** (2000) 67–72.
120. M. Eckert-Maksić, N. Novak-Doumbouya, R. Kiralj & B. Kojić-Prodić, "7-oxanorbornene Cycloadducts. X-ray, Molecular Orbital and Photoelectron Spectroscopic Study", *Journal of the Chemical Society-Perkin Transactions 2* (2000) 1483–1487.
119. V. Šverko, M. Radačić, M. Gavella, V. Lipovac, I. Ljubenković & M. Eckert-Maksić, "Effect of Cisplatin and 6-bromo-6-deoxy-L-ascorbic Acid on some Biochemical and Functional Parameters in Mice", *Toxicology* **137** (1999) 23–34.
118. M. Eckert-Maksić, I. Antol, M. Klessinger & Z. B. Maksić, "Proton Affinity of Substituted Naphthalenes", *Journal of Physical Organic Chemistry* **12** (1999) 597–604.
117. S. I. Kirin, F. G. Klärner & M. Eckert-Maksić, "High Pressure Synthesis of New Silicon Containing Heteroatom Analogues of Fused Norbornenes", *Synlett* (1999) 351–353.
116. Z. B. Maksić, I. Petanjek, M. Eckert-Maksić & I. Novak, "Ab Initio Study of Cyclobutadieno-*p*-benzoquinones: Kekulé Isomerization or not?", *Journal of Physical Chemistry A* **102** (1998) 10710–10714.
115. M. Eckert-Maksić, Z. Glasovac & Z. B. Maksić, "Molecular and Electronic Structure of Some Silacyclopropabenzene: The Reversed Mills-Nixon Effect", *Journal of Organometallic Chemistry* **571** (1998) 65–75.
114. S. I. Kirin, D. Vikić-Topić, E. Meštrović, B. Kaitner & M. Eckert-Maksić, "Diels-Alder Reactions of C-phenylated Siloles with 1,4-Epoxy-1,4-dihydronaphthalene", *Journal of Organometallic Chemistry* **566** (1998) 85–91.
113. M. Eckert-Maksić, A. Knežević & Z. B. Maksić, "Absolute Proton Affinities of Some Substituted Toluenes: The Additivity Rule of Thumb for *Ips*o Attack", *Journal of Physical Organic Chemistry* **11** (1998) 663–669.
112. I. Antol, M. Eckert-Maksić, D. Margetić, Z. B. Maksić, K. Kowski & P. Rademacher, "Molecular and Electronic Structure and Gas-Phase Pyrolytic Generation of 7,7'-Dioxasesquinorbornenes", *European Journal of Organic Chemistry* (1998) 1403–1408.
111. Z. B. Maksić, M. Eckert-Maksić & A. Knežević, "Methyl Cation Affinity vs Proton Affinity in Substituted Benzenes: An Ab Initio Study", *Journal of Physical Chemistry A* **102** (1998) 2981–2987.
110. M. W. Roomi, D. House, M. Eckert-Maksić, Z. B. Maksić & C. S. Tsao, "Growth Suppression of Malignant Leukemia Cell Line in vitro by Ascorbic Acid (Vitamin C) and its Derivatives", *Cancer Letters* **122** (1998) 93–99.
109. L. Moore, R. Lubinski, M. C. Baschky, G. D. Dahlke, M. Hare, T. Arrowood, Z. Glasovac, M. Eckert-Maksić & S. R. Kass, "Benzocyclopropenyl Anion: A Stable 8 π Electron Species", *Journal of Organic Chemistry* **62** (1997) 7390–7396.
108. M. Eckert-Maksić, M. Hodošček, D. Kovaček, Z. B. Maksić & M. Primorac, "Theoretical Model Calculations of the Absolute Proton Affinities of Benzonitrile, Nitroso- and Nitrobenzene", *Journal of Molecular Structure-Theochem* **417** (1997) 131–143.
107. M. Eckert-Maksić, M. Klessinger, I. Antol & Z. B. Maksić, "Additivity of Proton Affinities in Disubstituted Naphthalenes", *Journal of Physical Organic Chemistry* **10** (1997) 415–419.
106. M. Osmak, I. Kovaček, I. Ljubenković, R. Spaventi & M. Eckert-Maksić, "Ascorbic Acid and 6-Deoxy-6-chloro-Ascorbic acid: Potential Anticancer Drugs", *Neoplasma* **44** (1997) 101–107.
105. M. Eckert-Maksić, Lj. Maksimović, I. Zrinski, T. S. Kuznetsova & N. S. Zefirov, "Photoelectron Spectra and Conformational Behaviour of 3-Isopropenylcyclopropene Derivatives", *Croatia Chemica Acta* **69** (1996) 1521–1536.
104. M. Eckert-Maksić, Z. Glasovac, M. Hodošček, A. Lesar & Z. B. Maksić, "Molecular and Electronic Structure of 1,2-

- disilacyclobutabenzenes. *Ab Initio* Molecular Orbital and Density Functional Study", *Journal of Organometallic Chemistry* **524** (1996) 107–114.
103. Z. B. Maksić, M. Eckert-Maksić & M. Klessinger, "Additivity of the Proton Affinity of Polysubstituted Benzenes: The Ipso Position", *Chemical Physics Letters* **260** (1996) 572–576.
 102. M. Eckert-Maksić, M. Klessinger & Z. B. Maksić, "A Theoretical Study of the Additivity of Proton Affinities in Aromatics: Polysubstituted Benzenes", *Chemistry-a European Journal* **2** (1996) 1251–1257.
 101. Z. B. Maksić, D. Kovaček, M. Eckert-Maksić & I. Zrinski, "Theoretical Study of Additivity of the Deprotonation Energies in Aromatics. I. Disubstituted Benzenes", *Journal of Organic Chemistry* **61** (1996) 6717–6719.
 100. M. Eckert-Maksić, Z. Glasovac, Z. B. Maksić & I. Zrinski, "Electrophilic Reactivity in anti-Mills-Nixon Systems", *Journal of Molecular Structure-Theochem* **366** (1996) 173–183.
 99. C. Hillebrand, M. Klessinger, M. Eckert-Maksić & Z. B. Maksić, "Theoretical Model Calculations of the Proton Affinities of Aminoalkanes, Aniline, and Pyridine", *Journal of Physical Chemistry* **100** (1996) 9698–9702.
 98. M. Eckert-Maksić, M. Klessinger, D. Kovaček & Z. B. Maksić, "Model Calculations on the Electrophilic Reactivity of Fused Aromatics. Influence of the OH Substituent", *Journal of Physical Organic Chemistry* **9** (1996) 269–278.
 97. M. Eckert-Maksić, S. Elbel, M. Stohlmeier, S. Untiedt & A. de Meijere, "On the Effect of 1,2-disubstitution with Me₃M (M=Si, Ge, Sn) Groups upon the Electronic Structure of 3,3-dimethylcyclopropene", *Chemische Berichte* **129** (1996) 169–174.
 96. M. Eckert-Maksić, W. M. F. Fabian, R. Janoschek & Z. B. Maksić, "Theoretical Study of the Electrophilic Substitution Reactivity in Benzocyclobutadiene and Biphenylene", *Journal of Molecular Structure-Theochem* **338** (1995) 1–10.
 95. M. Eckert-Maksić, M. Klessinger & Z. B. Maksić, "Additivity of Proton Affinities: Theoretical Studies of Fluorine- and Methyl-Substituted Benzenes", *Journal of Physical Organic Chemistry* **8** (1995) 435–441.
 94. Z. B. Maksić, D. Kovaček, M. Eckert-Maksić, M. Bockmann & M. Klessinger, "Linear vs. Angular Phenylenes: An Interplay of Aromaticity, Antiaromaticity, and Baeyer Strain in Fused Molecular Systems", *Journal of Physical Chemistry* **99** (1995) 6410–6416.
 93. O. Mó, M. Yañez, M. Eckert-Maksić & Z. B. Maksić, "Bent Bonds in Benzocyclopropenes and their Fluorinated Derivatives", *Journal of Organic Chemistry* **60** (1995) 1638–1646.
 92. M. Eckert-Maksić, M. Golić & Lj. Paša-Tolić, "Photoelectron Spectroscopic Study of Novel Group 14 Functionalized Vinylcyclopropenes", *Journal of Organometallic Chemistry* **489** (1995) 35–41.
 91. M. Grdiša, M. Kralj, M. Eckert-Maksić, Z. B. Maksić & K. Pavelić, "6-Amino-6-Deoxyascorbic Acid Induces Apoptosis in Human Tumor-Cells", *Journal of Cancer Research and Clinical Oncology* **121** (1995) 98–102.
 90. M. Eckert-Maksić, M. Klessinger & Z. B. Maksić, "Theoretical Calculations of Proton Affinities in Phenol", *Chemical Physics Letters* **232** (1995) 472–478.
 89. M. Bonifačić, I. Ljubenkov & M. Eckert-Maksić, "One-Electron Oxidation and Reduction Reactions of Vitamin-C Derivatives: 6-Bromo and 6-Chloro-6-Deoxy-Ascorbic Acid", *International Journal of Radiation Biology* **66** (1994) 123–131.
 88. T. Bäcker, M. Klessinger, M. Eckert-Maksić & Z. B. Maksić, "The Relative Stability of the Tautomers of α -Hydroxytetronic Acid", *International Journal of Quantum Chemistry* **50** (1994) 385–394.
 87. M. Eckert-Maksić, Z. B. Maksić & M. Klessinger, "Protonation of Fused Aromatic Systems – *Ab Initio* Study of some Model Wheland Intermediates", *International Journal of Quantum Chemistry* **49** (1994) 383–396.
 86. M. Eckert-Maksić, Z. B. Maksić & M. Klessinger, "Theoretical-Study of Wheland Intermediates in Benzocycloalkenes - Vindication of the Mills-Nixon Hypothesis", *Journal of the Chemical Society-Perkin Transactions 2* (1994) 285–289.
 85. W. Koch, M. Eckert-Maksić & Z. B. Maksić, "Fluorination Effect on the Structural Properties in Benzocyclobutenes and Benzocyclobutadienes", *International Journal of Quantum Chemistry* **48** (1993) 319–332.
 84. Z. B. Maksić, M. Eckert-Maksić & K. H. Pfeifer, "Reversed Mills-Nixon Effect in Benzoborirene and Benzocyclopropenyl Cation", *Journal of Molecular Structure* **300** (1993) 445–453.
 83. M. Eckert-Maksić & M. Golić, "Thermally Induced Ring Opening of Novel Group 14 Functionalized Vinylcyclopropenes", *Journal of the Chemical Society-Perkin Transactions 2* (1993) 2325–2326.
 82. W. Koch, M. Eckert-Maksić & Z. B. Maksić, "Fluorination Effect on the Structural Properties of Selected Benzocyclopropenes", *Journal of the Chemical Society-Perkin Transactions 2* (1993) 2195–2202.
 81. M. Eckert-Maksić, D. Margetić, P. Rademacher & K. Kowski, "Photoelectron Spectroscopic Evidence for Formation of *syn*-7,7'-dioxasesquinorbornene", *Tetrahedron Letters* **34** (1993) 6951–6954.
 80. M. Eckert-Maksić, Z. B. Maksić, M. Hodošček & K. Poljanec, "The Mills-Nixon Effect in Trindan and Some Related Trisannulated Benzenes", *Journal of Molecular Structure-Theochem* **104** (1993) 187–194.
 79. M. Eckert-Maksić, Lj. Maksimović & M. Hodošček, "Electronic-Structure of Fused 7-Oxanorbornenes. Photoelectron Spectroscopic Study", *Tetrahedron Letters* **34** (1993) 4245–4248.
 78. M. Eckert-Maksić & D. Margetić, "Ionic Hydrogenation of Disubstituted Naphthalenes with BF₃·H₂O-Et₃SiH", *Energy & Fuels* **7** (1993) 315–318.
 77. J. E. Bloor, M. Eckert-Maksić, M. Hodošček, Z. B. Maksić & K. Poljanec, "*Ab Initio* Calculations of the Mills-Nixon Effect in Indan, Tetralin and in Related Systems", *New Journal of Chemistry* **17** (1993) 157–160.
 76. G. Baranović, M. Eckert-Maksić, M. Golić & J. R. Durig, "Vibrational Spectra, *Ab Initio* Calculations and Normal Coordinate Analysis for 3-methyl-3-Vinylcyclopropene", *Journal of Raman Spectroscopy* **24** (1993) 31–41.
 75. Lj. Maksimović, N. Novak & M. Eckert-Maksić, "Synthesis of some Novel Fused 7-Oxanorbornenes", *Synthetic Communications* **23** (1993) 3119–3125.
 74. D. Margetić, M. Eckert-Maksić & Z. B. Maksić, "Semiempirical Study of Isomerism and Intramolecular Hydrogen Bonds in some Substituted Anthraquinones", *Journal of Molecular Structure-Theochem* **96** (1992) 161–170.
 73. Z. B. Maksić, M. Eckert-Maksić, D. Kovaček & D. Margetić, "Strong Mills-Nixon Effect in Benzocyclobutadienes", *Journal of Molecular Structure-Theochem* **92** (1992) 241–248.
 72. Z. B. Maksić, D. Margetić & M. Eckert-Maksić, "A Semiempirical Study of Intramolecular Hydrogen-Bonding in some Naphthazarin Derivatives", *Croatica Chemica Acta* **65** (1992) 69–76.
 71. M. Eckert-Maksić, A. Lesar & Z. B. Maksić, "Fine Tuning of the Mills-Nixon Effect. Influence of Substituents in some 1,2-

- Dihydrobenzocyclobutenes and Benzocyclobutenes", *Journal of the Chemical Society-Perkin Transactions 2* (1992) 993–998.
70. M. Eckert-Maksić, Z. B. Maksić, M. Hodošček & K. Poljanec, "Mills-Nixon Effect in Heteroanalogues of Cyclopropabenzene", *International Journal of Quantum Chemistry* **42** (1992) 869–877.
 69. M. Eckert-Maksić, Z. B. Maksić, M. Hodošček & K. Rupnik, "Intra- and Extramolecular Electrostatic Potentials in Vitamin C", *Journal of Molecular Structure-Theochem* **88** (1992) 271–286.
 68. M. Eckert-Maksić, M. Hodošček & G. Fodor, "Theoretical-Study of (3,6)cyclohemiketal Form of L-Ascorbic Acid", *Croatica Chemica Acta* **64** (1991) 529–537.
 67. U. Höweler, T. Backer, M. Klessinger, M. Eckert-Maksić & Z. B. Maksić, "Theoretical-Studies of the Solvent Effect on the Stability of the Ascorbic Acid Tautomers", *Croatica Chemica Acta* **64** (1991) 539–549.
 66. Z. B. Maksić, M. Eckert-Maksić, D. Kovaček, M. Hodošček, K. Poljanec & J. Kudnig, "Is the Mills-Nixon Effect Operative in Perfluoro-Bezo(1,2:3,4:5,6)tricyclobutene?", *Journal of Molecular Structure-Theochem* **80** (1991) 201–212.
 65. M. Eckert-Maksić, S. Zollner, W. Göthling, R. Boese, Lj. Maksimović, R. Machinek & A. de Meijere, "Synthesis, Structure, and Electronic-Properties of Bis(tetramethylcyclopropylidene)methane and Bis(Cyclopropylidene)Methane", *Chemische Berichte-Recueil* **124** (1991) 1591–1596.
 64. M. Eckert-Maksić & Lj. Maksimović, "Long-Range Interaction Between Lone Pair Orbitals in Diepoxynaphthalene Derivatives", *Journal of Organic Chemistry* **56** (1991) 3719–3722.
 63. M. Eckert-Maksić & D. Margetić, "Ionic Hydrogenation of Organosulfur Compounds", *Energy & Fuels* **5** (1991) 327–332.
 62. M. Eckert-Maksić, R. Gleiter, N. S. Zefirov, S. I. Kozhushkov & T. S. Kuznetsova, "Photoelectron-Spectra of Geminal Vinyl- and Ethynyl-Disubstituted Cyclopropane Derivatives", *Chemische Berichte* **124** (1991) 371–376.
 61. M. Eckert-Maksić, M. Hodošček, D. Kovaček, Z. B. Maksić & K. Poljanec, "Strong Mills-Nixon Effect in Biphenylene", *Chemical Physics Letters* **171** (1990) 49–52.
 60. M. Eckert-Maksić, D. Kovaček, M. Hodošček, D. Mitić, K. Poljanec & Z. B. Maksić, "Mills-Nixon Effect in Benzocyclobutenes", *Journal of Molecular Structure-Theochem* **65** (1990) 89–98.
 59. Z. B. Maksić, M. Eckert-Maksić & D. Kovaček, "Semiempirical Study of Intramolecular Hydrogen Bond in Naphthazarin", *Croatica Chemica Acta* **62** (1990) 623–644.
 58. M. Eckert-Maksić, Z. B. Maksić & D. Margetić, "Semiempirical Study of Intramolecular Hydrogen Bond in 6-Hydroxy-2-Formylfulvene and 9-Hydroxyphenalenone", *Croatica Chemica Acta* **62** (1990) 645–660.
 57. M. Osmak, M. Eckert-Maksić, K. Pavelić, Z. B. Maksić, R. Spaventi, L. Beketić, I. Kovaček & B. Šuškić, "6-Deoxy-6-bromo-ascorbic Acid Inhibits Growth of Mouse Melanoma Cells", *Research in Experimental Medicine* **190** (1990) 443–449.
 56. Z. B. Maksić, M. Eckert-Maksić, P. N. Skancke & A. Skancke, "Protonation and Rehybridization. A Combined *Ab Initio* and Semiempirical Study", *Journal of Molecular Structure-Theochem* **46** (1988) 447–457.
 55. M. Eckert-Maksić, R. Gleiter, K. Hafner & H.-G. Klas, "The Electronic-Structure of 2-Azapentalenes. Photoelectron Spectroscopic Investigations", *Chemische Berichte-Recueil* **121** (1988) 1219–1223.
 54. M. Eckert-Maksić, Z. B. Maksić, A. Skancke & P. N. Skancke, "Structural Variations in Small Ring Hydrocarbons Bridged by Allenic Double Bonds", *Journal of Molecular Structure-Theochem* **41** (1988) 25–35.
 53. R. Gleiter, M. Eckert-Maksić & A. Konar, "The PE Spectra of the Seleno Analogues of Thieno [3,4-b]thiophene", *Chemische Berichte-Recueil* **120** (1987) 1917–1919.
 52. M. Eckert-Maksić & Lj. Maksimović, "Semiempirical MNDO Study of the Tautomerism in 3-substituted Tetronic Acids", *Journal of Molecular Structure-Theochem* **38** (1987) 121–131.
 51. M. Eckert-Maksić & Z. B. Maksić, "Semiempirical vs. *Ab Initio* Calculations of Molecular Properties: Part 4. Nuclear-Quadrupole Coupling-Constants of ¹⁴N in some Medium-Sized Heterocyclic Molecules", *Journal of Molecular Structure-Theochem* **38** (1987) 133–139.
 50. M. Eckert-Maksić, Z. B. Maksić, A. Skancke & P. N. Skancke, "Geometric Structure and Energetics of Small Strained Hydrocarbons Involving an *Exo*-double Bond: A Combined Semiempirical and *Ab Initio* Study", *Journal of Physical Chemistry* **91** (1987) 2786–2790.
 49. M. Eckert-Maksić, K. Mlinarić-Majerski & Z. Majerski, "Electronic Structure of 2,4-Methano-2,4-didehydroadamantane: A [3.1.1]propellane. Photoelectron and Semiempirical Studies", *Journal of Organic Chemistry* **52** (1987) 2098–2100.
 48. A. Skancke, P. N. Skancke, M. Eckert-Maksić & Z. B. Maksić, "Vibrational Force Fields for Strained Hydrocarbons Involving *exo*-Double Bonds. An *Ab Initio* Study", *Journal of Molecular Structure-Theochem* **35** (1987) 259–266.
 47. C. F. Wilcox, D. A. Blain, J. Clardy, G. van Duynne, R. Gleiter & M. Eckert-Maksić, "3*H*-Cyclonona[*def*]biphenylene: An example of Neutral Homoantiaromaticity", *Journal of the American Chemical Society* **108** (1986) 7693–7702.
 46. M. Eckert-Maksić, P. Bischof & Z. B. Maksić, "On the Stability of Vitamin C radicals", *Zeitschrift Fur Naturforschung Section a-a Journal of Physical Sciences* **41** (1986) 1315–1318.
 45. M. Eckert-Maksić, P. Bischof & Z. B. Maksić, "Geometric and Electronic Structure of Vitamin C Radicals. A Semiempirical Study", *Journal of Molecular Structure-Theochem* **32** (1986) 179–195.
 44. N. S. Zefirov, S. I. Kozhushkov, T. S. Kuznetsova, R. Gleiter & M. Eckert-Maksić, "Synthesis of gem-Disubstituted Ethylene and Acetylene Derivatives of the Cyclopropane Series Based on 1,1-Diacetylcyclopropanes", *Russian Journal of Organic Chemistry* **22** (1986) 95–105.
 43. M. Eckert-Maksić & R. Gleiter, "Photoelectron-Spectra of N-Substituted 1,4-Dihydro-4,4-dimethylpyridines", *Chemische Berichte* **119** (1986) 2381–2386.
 42. M. Eckert-Maksić & Lj. Maksimović, "MNDO Study of Tautomerism in 3-Acetyltetramic Acid", *Croatica Chemica Acta* **59** (1986) 757–767.
 41. H. U. Hofs, J. W. Bats, R. Gleiter, G. Hartmann, R. Mews, M. Eckert-Maksić, H. Oberhammer & G. M. Sheldrick, "Perhalogenated 1,2,3,5-Dithiadiazolium Salts and 1,2,3,5-Dithiadiazoles", *Chemische Berichte-Recueil* **118** (1985) 3781–3804.
 40. M. Eckert-Maksić & Z. B. Maksić, "Semiempirical MNDO Study of Phenyl-Sydnone and its Protonated Forms", *Croatica Chemica Acta* **58** (1985) 15–27.
 39. M. Eckert-Maksić, P. Bischof & Z. B. Maksić, "Vitamin-C and its Radicals. Tautomerism, Electronic-Structure and Properties", *Croatica Chemica Acta* **58** (1985) 407–426.
 38. Z. B. Maksić, M. Eckert-Maksić & K. Rupnik, "Model Description of Some Molecular Properties by the Modified Atom-In-Molecule (MAM) Approach", *Croatica Chemica Acta* **57** (1984) 1295–1353.

37. R. Gleiter, W. Dobler, M. Eckert-Maksić, A. J. Bloodworth, H. J. Eggelte & D. Cremer, "Photoelectron-Spectra of Dioxabicyclo[n.2.1]alkanes", *Journal of Organic Chemistry* **49** (1984) 3716–3720.
36. M. Eckert-Maksić, Z. B. Maksić & R. Gleiter, "A Comparative Study of Bent-Bond vs. Walsh Model in Strained Systems. Bicyclo[1.1.0]butane", *Theoretica Chimica Acta* **66** (1984) 193–205.
35. M. Eckert-Maksić, "Protonation of 4H-Pyran-4-one and its Sulfur Analogs. MNDO Study", *Zeitschrift Für Naturforschung Section a-a Journal of Physical Sciences* **39** (1984) 267–275.
34. R. Gleiter, R. W. Saalfrank, W. Paul, D. O. Cowan & M. Eckert-Maksić, "The Photoelectron Spectrum of 1,1-Diethoxy-3,3-bis(trifluoromethyl)allene. The Effect of Trifluoromethyl Groups on Cumulative Systems", *Chemische Berichte-Recueil* **116** (1983) 2888–2895.
33. R. Gleiter, M. C. Böhm, M. Eckert-Maksić, W. Schäfer, M. Baudler, Y. Aktalay, G. Fritz & K. D. Hoppe, "The Electronic-Structure of Phosphorus Cages with the Nortricyclane Skeleton. - Model Calculations and Photoelectron Spectroscopic Investigations", *Chemische Berichte-Recueil* **116** (1983) 2972–2982.
32. Z. B. Maksić & M. Eckert-Maksić, "Geometry of Molecules. Part 6. Interatomic Distances and Electronic Structures of Some Alkylsubstituted 4-Membered and 5-Membered Cyclic Hydrocarbons", *Journal of Molecular Structure-Theochem* **8** (1983) 295–311.
31. R. Gleiter, W. Dobler & M. Eckert-Maksić, "How Similar are Tropoquinones and Benzoquinone?", *Angewandte Chemie-International Edition in English* **21** (1982) 76–76.
30. M. C. Böhm, M. Eckert-Maksić, R. Gleiter, G. E. Herberich & B. Hessner, "Die Elektronenstruktur und das He(I)-Photoelektronen-Spektrum von (Cyclopentadienyl)(1,4-dimethyl-1,4-dibora-2,5-cyclohexadien)cobalt", *Chemische Berichte-Recueil* **115** (1982) 754–763.
29. R. Gleiter, M. Eckert-Maksić, W. Schafer & E. A. Truesdale, "Quest for a Strong Through Bond Interaction in [2.2]Paracyclophane", *Chemische Berichte-Recueil* **115** (1982) 2009–2011.
28. J. Spanget-Larsen, C. de Korsewagen, M. Eckert-Maksić & R. Gleiter, "Electronic and Molecular-Structure of Simple 3,3'-Bicyclopropenyls. Photoelectron Spectroscopy and Model-Calculations", *Helvetica Chimica Acta* **65** (1982) 968–982.
27. M. C. Böhm, M. Eckert-Maksić, R. D. Ernst, D. R. Wilson & R. Gleiter, "Electronic-Structure of Organo-Metallic Compounds. 18. Electronic-Structure of Bis(pentadienyl)iron. Semiempirical Calculations and Photoelectron Spectra", *Journal of the American Chemical Society* **104** (1982) 2699–2707.
26. R. Gleiter, W. Dobler & M. Eckert-Maksić, "The Electronic-Structure of *o*-Tropoquinone, *p*-Tropoquinone and Cyclopentene-1,2,3-trione. PE Spectroscopic Investigations", *Nouveau Journal De Chimie-New Journal of Chemistry* **6** (1982) 123–127.
25. M. Eckert-Maksić & Z. B. Maksić, "Geometry of Molecules. Part 5. Interatomic Distances and Electronic-Structures of Some Alkylsubstituted Cyclopropanes and Cyclopropenes by the IMO Method", *Theochem-Journal of Molecular Structure* **3** (1982) 325–340.
24. M. Eckert-Maksić, "MINDO/3 Study of the Protonation of Phenol and Methylphenols", *Zeitschrift Fur Naturforschung Section a-a Journal of Physical Sciences* **37** (1982) 688–696.
23. M. C. Böhm, M. Eckert-Maksić, R. Gleiter, J. Grobe & D. Le Van, "The He(I) Photoelectron Spectra of (CH₃)₂PSCH₃, (CH₃)₂AsSCH₃, (CH₃)₂AsSeCH₃ and (CH₃)₂PSeCH₃", *Chemische Berichte-Recueil* **114** (1981) 2300–2308.
22. R. Gleiter, W. Schäfer & M. Eckert-Maksić, "Trans-Annular Interactions Between Acetylenes - Photoelectron Spectroscopic Investigations on 1,8-Diethynyl-naphthalene and Cyclic-Derivatives of 2,2'-Diethynylbiphenyl", *Chemische Berichte-Recueil* **114** (1981) 2309–2321.
21. R. Gleiter, K. Gubernator, M. Eckert-Maksić, J. Spanget-Larsen, B. Bianco, G. Gandillon & U. Burger, "The Electronic-Structure of Phenylene and Naphthylene Bicyclobutanes. Photoelectron-Spectroscopy and Model Calculations", *Helvetica Chimica Acta* **64** (1981) 1312–1321.
20. M. Eckert-Maksić, "Protonation of Alkyl Aryl Sulfides in Antimony Pentafluoride-Fluorosulfonic Acid-Solution", *Journal of the Chemical Society-Perkin Transactions 2* (1981) 62–64.
19. M. Eckert-Maksić & Z. B. Maksić, "MNDO Study of the Site of Protonation in Methylsydnone", *Journal of the Chemical Society-Perkin Transactions 2* (1981) 1462–1466.
18. P. Bischof, M. Eckert-Maksić & Z. B. Maksić, "On The Relative Stability of Ascorbic-Acid Tautomers", *Zeitschrift Für Naturforschung Section a-a Journal of Physical Sciences* **36** (1981) 502–504.
17. H. D. Martin, M. Eckert-Maksić & B. Mayer, "Small Rings Diagonal Interaction in the 4-Membered Ring. Experimental Demonstration of a Dominating Circumannular Conjugation: 5,6-Dimethylenebicyclo[2.1.1]hexane", *Angewandte Chemie-International Edition in English* **19** (1980) 807–809.
16. R. Gleiter, H. Hopf, M. Eckert-Maksić & K. L. Noble, "Photoelectron-Spectra of [8]Paracyclophane and [8]Paracyclophane-4-Ene. An Estimation of Inductive and Hyperconjugative Effect for N-Paracyclophanes", *Chemische Berichte-Recueil* **113** (1980) 3401–3403.
15. M. Eckert-Maksić, "Protonation of Methoxyphenyl Alkyl Sulfides in Pentafluoroantimony-Fluorosulfonic Acid", *Journal of Organic Chemistry* **45** (1980) 3355–3357.
14. Z. B. Maksić, K. Rupnik & M. Eckert-Maksić, "Semiempirical Studies of Core Electron Binding Energy Shifts V. SCC-MO Investigation of Keto-Enol Tautomerism in Some 1,3-Diketones and Related Anhydrides", *Journal of Electron Spectroscopy and Related Phenomena* **16** (1979) 371–377.
13. M. Eckert-Maksić, K. Kovačević & Z. B. Maksić, "Electronic-Structure of Organosilicon Compounds. III. Iterative Maximum Overlap Calculations on Some Cyclic and Polycyclic Silanes", *Journal of Organometallic Chemistry* **168** (1979) 295–310.
12. Z. B. Maksić, K. Kovačević & M. Eckert-Maksić, "Calculation of Strain Energies in Cyclic and Polycyclic-Hydrocarbons by Maximum Overlap Approximation", *Tetrahedron Letters* **16** (1975) 101–104.
11. K. Kovačević, M. Eckert-Maksić & Z. B. Maksić, "Calculation of Heats of Formation, Heats of Hydrogenation and Strain Energies in Nonconjugated Hydrocarbons by Maximum Overlap Approximation", *Croatica Chimica Acta* **46** (1974) 249–259.
10. M. Eckert-Maksić & Z. B. Maksić, "Maximum Overlap Hybridization in Norbornane and Some Related Molecules", *Journal of Molecular Structure* **22** (1974) 445–456.
9. K. Kovačević, M. Eckert-Maksić & Z. B. Maksić, "Calculation of Heats of Formation in Some Cyclic and Polycyclic Hydrocarbons by MOA Method", *Journal of Molecular Structure* **21** (1974) 335–337.
8. J. W. Larsen & M. Eckert-Maksić, "Ambident Behavior of Some Phenols and Alkoxybenzenes in Antimony Pentafluoride-Fluorosulfonic acid Mixtures", *Journal of the American Chemical Society* **96** (1974) 4311–4316.
7. J. W. Larsen & M. Eckert-Maksić, "Structures of Protonated Methyl Phenols in Antimony Pentafluoride-Fluorosulfuric Acid at -60 °C", *Croatica Chimica Acta* **45** (1973) 503–510.

6. J. W. Larsen & M. Eckert-Maksić, "p-Methylanisole as an Ambident Base - Effect of Acid Strength on Position of Protonation", *Tetrahedron Letters* **13** (1972) 1477–1480.
5. Z. B. Maksić, M. Eckert-Maksić & M. Randić, "Correlation between C-H and C-C Spin-Spin Coupling Constants and s-character of Hybrids Calculated by Maximum Overlap Method", *Theoretica Chimica Acta* **22** (1971) 70–79.
4. M. Eckert-Maksić, L. Tušek & D. E. Sunko, "Rates of Oxidation of Some Bicyclic Alcohols with Silver Carbonate on Celite", *Croatica Chemica Acta* **43** (1971) 79–81.
3. M. Eckert-Maksić, Z. Majerski, S. Borčić & D. E. Sunko, "Competitive Reactions of Nucleophiles. II. Solvolysis of α,α - and γ,γ -Dimethylallyl Chlorides", *Tetrahedron* **27** (1971) 2119–2124.
2. Z. B. Maksić & M. Eckert-Maksić, "Some Remarks on the Use of Experimental Bond Lengths in the Maximum Overlap Method", *Croatica Chemica Acta* **42** (1970) 433–449.
1. Z. B. Maksić & M. Eckert-Maksić, "A Correlation between Acidity and Hybridization in Non-Conjugated Hydrocarbons", *Tetrahedron* **25** (1969) 5113–5114.

Review Papers and Book Chapters

12. M. Barbatti, M. Ruckebauer, J. J. Szymczak, B. Sellner, M. Vazdar, I. Antol, M. Eckert-Maksić & H. Lischka, "Model Systems for dynamics of π -conjugated Molecules in the Excited States", *Vademecum of Computational Chemistry* (M. Shukla, J. Leszczynski, Eds.), Springer 2011, 1175–1213.
11. M. Eckert-Maksić, I. Antol, M. Vazdar, M. Barbatti & H. Lischka, "Formamide as the Model Compound for Photodissociation Studies of the Peptide Bond" in "Kinetics and Dynamics: From Nano- to Bio-Scale" (P. Paneth, A. Dybala-Defratyka, Eds.), Springer, 2010, 77–107.
10. M. Eckert-Maksić & Z. B. Maksić, "Antiaromaticity and Aromaticity in Carbocyclic Four-membered Rings" in "The Chemistry of Cyclobutenes", Z. Rappoport, J. F. Liebmann (Eds.), J. Wiley&Sons, 2005, 17–82.
9. Z. B. Maksić, M. Eckert-Maksić, O. Mó & M. Yañez, "The Mills-Nixon Effect: Fallacies, Facts and Chemical Relevance" in: "Theoretical and Computation Chemistry", Z. B. Maksić, (Ed.), Elsevier (1998) 47–101.
8. Z.B. Maksić & M. Eckert-Maksić, "Intrinsic Proton Affinity of Substituted Aromatics" in "Theoretical Organic Chemistry", C. Parkanyi, (Ed.), Elsevier (1997) 203–235.
7. M. Eckert-Maksić, "Photoelectron Spectroscopy of Alcohols, Phenols, Ethers and Peroxides" in: "Chemistry of Hydroxyl, Ether and Peroxides Group", S. Patai (Ed.), J. Wiley, Suppl. E2 1993, 299–371.
6. M. Eckert-Maksić, "Through-space and Through-bond Interactions as Mirrored by Photoelectron Spectroscopy" in: "Theoretical Models of Chemical Bonding", Z. B. Maksić (Ed.), Springer Verlag, 1991, 153–198.
5. Z.B. Maksić, M. Eckert-Maksić, M. Hodošček, W. Koch & D. Kovaček, "Theoretical Studies of the Mills-Nixon Effect", in: "Molecules in Natural Science and Medicine. An Encomium for Linus Pauling", Z.B. Maksić and M. Eckert-Maksić, (Eds.), Ellis Horwood, Chichester, 1991, 333–349.
4. M. Eckert-Maksić, I. Kovaček, Z. B. Maksić, M. Osmak & K. Pavelić, "Effect of Ascorbic Acid and its Derivatives on Different Tumors in vitro and in vivo", in: "Molecules in Natural Science and Medicine. An Encomium for Linus Pauling", Z.B. Maksić and M. Eckert-Maksić, (Eds.), Ellis Horwood, Chichester, 1991, 509–524.

Scientific Conference Papers with International Peer-review

2. I. Kovaček, M. Osmak, R. Spaventi & M. Eckert-Maksić, "Inhibitory Effect of L-Ascorbic Acid and 6-Deoxy-6-chloro Ascorbic Acid on the Growth of Human Tumor Cells in vitro", Proceedings of the Croatian-Slovenian Meeting, M. Osmak, J. Škrk (Eds.), Zagreb (1996), pp. 165–168.
1. G. Baranović, M. Eckert-Maksić, L. Balta, D. Kovaček & K. Furić, "Raman Study of the Vibrational Spectrum and Rotational Isomerism of 3-methyl-3-vinyl-cyclopropene", Proceedings of the XII. International conference on Raman Spectroscopy, J. R. Durig, J. F. Sullivan (Eds.), John Wiley & Sons, 1990, p. 94.

Electronic Conference Papers

5. Z. Glasovac, M. Vazdar, M. Eckert-Maksić & D. Margetić, "Proton Affinities of Dehydroporphyrin and Subporphyrin in Ground and Excited States Obtained by High Level Computations", The eleventh electronic computational chemistry conference (ECCC-11, R. Q. Topper, Ed.), 2007.
4. D. Margetić, M. Vazdar & M. Eckert-Maksić, "Syn-2,7-disilatetracyclo[6.2.1.1^{3,6}0^{2,7}]dodec-2(7)-ene: Structural Influence of Incorporation of Disilene into Sesquinorbornene Framework: A DFT Study." *Int. Electron. J. Mol. Des.* **4** (2005) 647–658.
3. D. Margetić, M. Eckert-Maksić & S. Kirin, "High Pressure Assisted Synthesis of Fused Norbornenes Containing Two 7-Metallonorbornene Units", Proceedings of 8th Electronic Conference on Synthetic Organic Chemistry (ECSOC-8, J. A. Seijas Vazquez, S.-K. Lin, D. C. Ji, Eds., Basel, MDPI, 2004).
2. D. Margetić & M. Eckert-Maksić, "High Pressure Synthesis of oOrganometallic Norbornene Derivatives and Semiempirical Quantum-Chemical Study of Reactivity of Cyclic Organometallic Dienes", Proceedings of 7th Electronic Conference on Synthetic Organic Chemistry (ECSOC-7 (Ed. J. A. Seijas, De-chun Ji and Shu-Kun Lin), Base, M DPI, 2003).
1. D. Margetić, R. N. Warrener, M. Eckert-Maksić, I. Antol & Z. Glasovac, "A DFT Study of Pyramidalized Alkenes: 7-Oxasesquinorbornenes and 7,7-dioxasesquinorbornenes", The Eight Electronic Computational Chemistry Conference (ECCC-8, R. Q. Topper, Ed.), 2002.

Book and Conference Abstract Editing

3. Book of Abstracts "8th European Symposium on Organic Reactivity" (M. Eckert-Maksić, Z. Glasovac, I. Zrinski, Eds.), Zagreb, 2001.
2. "Kako živjeti dulje i osjećati se bolje", (translation of the L. Paulings book "How to leave longer and feel better"), together with Z. B. Maksić, Globus, I. Ed.1989, II. Ed. 1990, III. Ed. 1997.
1. "Molecules in Natural Science and Medicine" (Z. B. Maksić, i M. Eckert-Maksić, Eds.), Elsevier, 1992.

5. M. Eckert-Maksić, "Chemistry in Croatia", *Nachrichten aus der Chemie* **49** (2001) 05, 627–630.
4. S. I. Kirin & M. Eckert-Maksić, "Sinteza organskih spojeva pod visokim tlakom", *Kemija u industriji* **48** (1999) 335–343
3. M. Eckert-Maksić, Z. B. Maksić, M. Osmak & K. Pavelić, "Vitamin C - Struktura, biološka svojstva i reaktivnost", *Kemija u industriji* **43** (1994) 461–473.
2. M. Eckert-Maksić & Z. B. Maksić, "Ta izvanredna molekula vitamin C", *Priroda* **10** (1988/89) 21–23.
1. M. Eckert-Maksić, "Superkiseline u kemiji", *Kemija u industriji* **30** (1981) 129–136.

Professional and Popular Papers

8. M. Eckert-Maksić, "Institut Ruđer Bošković", Leksikon Ruđera Boškovića, Leksikografski zavod Miroslav Krleža, Ed: A. Bogutovac, Zagreb 2011, pp. 52–55.
7. M. Eckert-Maksić, "Svečana proslava 60. obljetnice Instituta Ruđer Bošković", *Kemija u industriji* **59** (2010), 624–626.
6. I. Zrinski & M. Eckert-Maksić, "Primjena mikrovalnog zračenja u organskoj sintezi", *Kemija u industriji* **54** (2005), 469–476.

Patent Applications and Patents

3. M. Maksić & Z. Glasovac, Pat. Appl. HR P20040341 A2, 2005; PCT/HR 2005/000026, Patent: EP 1786 763.
2. M. Maksić & I. Ljubenkov, Pat. Appl., Zagreb, Republic of Croatia, 1998 (HP-P980102A)
1. M. Maksić & I. Ljubenkov, Pat. Appl., Zagreb, Republic of Croatia, 1998 (HP-P980542A).