

## 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 II(N)–Σ(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 (8π,6π)-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.
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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.
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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.
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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.
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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.
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