

LIST OF PUBLICATIONS

172. T. Kireilis, K. J. Szabó*: Stereoselective Copper-Catalyzed Cross-Coupling of α -CF₃-Allylboronic Acids with Diazoketones. *J. Org. Chem.* **2025**, DOI: [10.1021/acs.joc.4c02869](https://doi.org/10.1021/acs.joc.4c02869).
171. K. Bajerke, F. Lehmann, G. Antoni, K. J. Szabó* ¹⁸F-Labeling of Nitrogen-containing Aryl Boronates – Anti-cancer Drug Melflufen as a Case Study. *Org. Chem. Front.* **2024**, *11*, 6411-6417.
170. M. Biosca, F. Himo,* K. J. Szabó*: Mechanism of Asymmetric Homologation of Alkenylboronic Acids with CF₃-Diazomethane via Borotropic Rearrangement. *J. Org. Chem.* **2024**, *89*, 4538-4548.
169. M. Deliaval, R. Jayarajan, L. Eriksson, K. J. Szabó*: Three-Component Approach to Densely Functionalized Trifluoromethyl Allenols by Asymmetric Organocatalysis. *J. Am. Chem. Soc.* **2023**, *142* 10001-10006. Highlighted in Synfacts: B. List, W. Leinung, BINOL Catalysis Permits One-Pot Synthesis of Chiral Trifluoromethyl and Trimethylsilyl Allenols; *Synfacts* **2023**, *19*, 0710.
168. Q. Wang, L. Eriksson, K. J. Szabó*: Catalytic Homologation-Allylboration Sequence for Diastereo- and Enantioselective Synthesis of Densely Functionalized β -Fluorohydrins with Tertiary Fluoride Stereocenters. *Angew. Chem. Int. Ed. (Hot Paper)*, **2023**, *62* e202301481.
167. Q. Wang, T. Nilsson, L. Eriksson, K. J. Szabó*: Sulfenofunctionalization of Chiral α -Trifluoromethyl Allylboronic Acids: Asymmetric Synthesis of SCF₃, SCF₂R, SCN and SAR Compounds. *Angew. Chem. Int. Ed.*, **2022**, *61*, e202210509.
166. R. Jayarajan, T. Kireilis, L. Eriksson, K. J. Szabó*: Asymmetric Organocatalytic Homologation: Access to Diverse Chiral Trifluoromethyl Organoboron Species. *Chem. Eur. J.* **2022**, *28* e202202059.
165. Q. Wang, M. Biosca, F. Himo,* K. J. Szabó*: Electrophilic Fluorination of Alkenes via Bora-Wagner-Meerwein Rearrangement. Access to β -Difluoroalkyl Boronates. *Angew. Chem. Int. Ed. (Hot Paper)* **2021**, *60*, 26327-26331. Highlighted in Synfacts: List, B.; Mitschke, B. An Aryl Iodide Catalyzed Bora-Wagner-Meerwein Rearrangement; *Synfacts* **2021**, *17*, 1383.
164. D. N. Meyer, M. A. Cortés González, X. Jiang, L. Johansson-Holm, M. Pourghasemi Lati, M. Elgland, P. Nordeman, G. Antoni, K. J. Szabó*: Base-catalysed ¹⁸F-Labeling of Trifluoromethyl Ketones. Application to the Synthesis of ¹⁸F-Labelled Neutrophil Elastase Inhibitors. *Chem. Commun.* **2021**, *57*, 8476-8479.
163. K. J. Szabó*: Fluorination, trifluoromethylation and trifluoromethylthiolation of alkenes, cyclopropanes and diazo compounds. In "Organofluorine Chemistry: Synthesis, Modeling, and Applications" K. J. Szabó, N. Selander, Eds. *Wiley-VCH* **2021**, Chapter 6, 201-223.
162. Organofluorine Chemistry: Synthesis, Modeling, and Applications. K. J. Szabó, N. Selander, Eds. Wiley-VCH, **2021**, ISBN: 978-3-527-82514-1

161. S. J. T. Jonker[§], R. Jayarajan[§], T. Kireilis, M. Deliaval, L. Eriksson, K. J. Szabó*: Organocatalytic Synthesis of α -Trifluoromethyl Allylboronic Acids by Enantioselective 1,2-Borotropic Migration; [J. Am. Chem. Soc. 2020, 142, 21254-21259](#). [§]Contributed equally.
160. Q. Wang[§], M. Lübcke[§], M. Biosca[§], M. Hedberg, L. Eriksson, F. Himo*, K. J. Szabó*: Enantioselective Construction of Tertiary Fluoride Stereocenters by Organocatalytic Fluorocyclization; [J. Am. Chem. Soc. 2020, 142, 20048-20057](#). [§]Contributed equally. Highlighted in Synfacts: B. List, S. Brunen, S: Hypervalent Iodine Triggers Asymmetric Fluorocyclization toward Tertiary C–F Stereocenters; [Synfacts 2021, 17, 0209](#).
159. O. Brea, K. J. Szabó*, F. Himo*: Mechanisms of Formation and Rearrangement of Benziodoxole-Based CF₃ and SCF₃ Transfer Reagents; [J. Org. Chem. 2020, 85, 15577-15585](#).
158. M. Lübcke, K. J. Szabó*: Diazocarbonyl Compounds in Organofluorine Chemistry; [Synlett 2021, 32, 1060-1071](#).
157. X. Jiang, D. Meyer, D. Baran, M. A. Cortés González, K. J. Szabó*: Trifluoromethylthiolation, Trifluoromethylation and Arylation Reactions of Difluoro Enol Silyl Ethers [J. Org. Chem. 2020, 85, 8311–8319](#). Highlighted in [JOC 2020 Featured Articles: Unique, Inspiring, and Exceptionally Well-Done Chemistry](#).
156. M. A. Cortés Gonzáles; X. Jiang, P. Nordeman, G. Antoni, K. Szabó*: Rhodium-mediated 18F-oxyfluorination of diazoketones using fluorine-18-containing hypervalent iodine reagent. [J. Chem. Commun. 2019, 55, 13358-13361](#).
155. S. Agasti, B. Mondal, T. K. Achar, S. K. Sinha, A. Sarala-Suseelan, K. J. Szabó,* F. Schoenebeck,* D. Maiti,* [ACS Catal. 2019, 9, 9606-9613](#).
154. M. Lübcke, D. Bezhan, K. J. Szabó*: Trifluoromethylthiolation-Arylation of Diazocarbonyl Compounds by Modified Hooz Multicomponent Coupling. [Chem. Sci. 2019, 10, 5990-5995](#).
153. S. J. T. Jonker, C. Diner, G. Schulz, H. Iwamoto, L. Eriksson, K. J. Szabó*: Catalytic asymmetric propargyl- and allylboration of hydrazonoesters: a metal-free approach to sterically encumbered chiral α -amino acid derivatives. [Chem. Commun., 2018, 54, 12852-12855](#).
152. B. K. Mai, K. J. Szabó,* F. Himo*: Mechanisms of Rh-Catalyzed Oxyaminofluorination and Oxyaminotrifluoromethylthiolation of Diazocarbonyl Compounds with Electrophilic Reagents. [Org. Lett. 2018, 20, 6646-6649](#).
151. D. Wang, M. J. M. de Wit, K. J. Szabó*: Synthesis of Densely Substituted Conjugated Dienes by Transition-metal-free Reductive Coupling of Allenylboronic Acids and Tosylhydrazones. [J. Org. Chem. 2018, 83, 8786-8792](#).
150. B. K. Mai, K. J. Szabó,* F. Himo*: Mechanisms of Rh-Catalyzed Oxyfluorination and Oxytrifluoromethylation of Diazocarbonyl Compounds with Hypervalent Fluoroiodine. [ACS Catal. 2018, 8, 4483-4492](#).

149. M. A. Cortes Gonzalez, P. Nordeman, A. Bermejo Gomez, D. N. Meyer, G. Antoni, M. Schou, K. J. Szabó*: [¹⁸F]Fluoro-benziodoxole: A no-carrier-added electrophilic fluorinating reagent. Rapid, simple radiosynthesis, purification and application for fluorine-18 labelling. *Chem. Commun.* **2018**, *54*, 4286-4289.
148. J. Zhao, S. J. T. Jonker, D. N. Meyer, G. Schulz, C. D. Tran, L. Eriksson, K. J. Szabó*: Copper-Catalyzed Synthesis of Allenylboronic Acids. Access to Sterically Encumbered Homopropargylic Alcohols and Amines by Propargylboration. *Chem. Sci.* **2018**, *9*, 3305-3312.
147. L. T. Pilarski, K. J. Szabó*: Catalysis with Transition Metal Pincer Complexes. In *Applied Homogenous Catalysis with Organometallic Compounds*. Eds. B. Cornils, W. A. Hermann, M. Beller, R. Paciello. **2018**, Vol. 3, 889-898. Wiley-VCH.
146. L. Mao, R. Bertermann, S. G. Rachor, K. J. Szabó,* T. B. Marder*: Palladium-Catalyzed Oxidative Borylation of Allylic C–H Bonds in Alkenes. *Org. Lett.* **2017**, *19*, 6590-6593.
145. L. Mao, R. Bertermann, K. Emmert, K. J. Szabó,* T. B. Marder*: Synthesis of Vinyl-, Allyl-, and 2-Boryl Allylboronates via a Highly Selective Copper-Catalyzed Borylation of Propargylic Alcohols. *Org. Lett.* **2017**, *19*, 6586-6589.
144. G. Huang, C. Diner, K. J. Szabó,* F. Himo*: Mechanism and Stereoselectivity of the BINOL-Catalyzed Allylboration of Skatoles. *Org. Lett.* **2017**, *19*, 5904-5907.
143. M. Lübcke, W. Yuan, K. J. Szabó*: Trifluoromethylthiolation-Based Bifunctionalization of Diazocarbonyl Compounds by Rhodium Catalysis. *Org. Lett.* **2017**, *19*, 4548-4551.
142. N. O. Ilchenko, K. J. Szabó*: Geminal difluorination of α,α' -disubstituted styrenes using fluoro-benziodoxole reagent. Migration aptitude of the α -substituents. *J. Fluor. Chem.* **2017**, *203*, 104-109.
141. D. Wang, K. J. Szabó*: Copper-Catalyzed, Stereoselective Cross-Coupling of Cyclic Allyl Boronic Acids with α -Diazoketones *Org. Lett.* **2017**, *19*, 1622-1625.
140. L. Mao, K. J. Szabó*; T. B. Marder*: Synthesis of Benzyl-, Allyl-, and Allenylboronates via Copper-Catalyzed Borylation of Alcohols *Org. Lett.* **2017**, *19*, 1204-1207.
139. N. O. Ilchenko, M. Hedberg, K. J. Szabó*: Fluorinative Ring-opening of Cyclopropanes by Hypervalent Iodine Reagents. An Efficient Method for 1,3-Oxyfluorination and 1,3-Difluorination. *Chem. Sci.* **2017**, *8*, 1056-1061.
138. A. Bermejo Gomez,* M. Cortes, M. Lübcke, M. Johansson, M. Schou, K. J. Szabó*: Synthesis of Trifluoromethyl Moieties by Late-stage Copper(I) Mediated Nucleophilic fluorination. *J. Fluor. Chem.* **2017**, *194*, 51-57.
137. J. Zhang, K. J. Szabó,* F. Himo*: Metathesis Mechanism of Zinc-Catalyzed Fluorination of Alkenes with Hypervalent Fluoroiodine. *ACS Catal.* **2017**, *7*, 1093-1100.

136. D. Colin, K. J. Szabó*: Recent Advances in the Preparation and Application of Allylboron Species in Organic Synthesis. *J. Am. Chem. Soc.* **2017**, *139*, 2-14. (Highlighted in Spotlights on Recent JACS Publications *J. Am. Chem. Soc.* **2017**, *139*, 1)
135. A. Bermejo Gomez, M. Cortes, M. Lübcke, M. Johansson, C. Halldin, K. J. Szabó,* M. Schou*: Efficient DBU accelerated synthesis of ¹⁸F-labelled trifluoroacetamides. *Chem. Commun.* **2016**, *52*, 13963-13966.
134. R. Alam, C. Diner, S. Jonker, K. J. Szabó*: Catalytic Asymmetric Allylboration of Indoles and Dihydroisoquinolines with Allylboronic Acids. Stereodivergent Synthesis up to Three Contiguous Stereocenters. *Angew. Chem. Int. Ed.* **2016**, *55*, 14417-14421. (Highlighted in *Chemistry Views*; *Synfacts*, *Chemistry World*, and *Angewandte's Personal Profile*)
133. W. Yuan, K. J. Szabó*: Rhodium-Catalyzed Oxy-Aminofluorination of Diazoketones with Tetrahydrofurans and NFSI. *ACS Catal.* **2016**, *6*, 6687-6691.
132. M.-C. Belhomme, D. Wang, K. J. Szabó*: Formation of C(sp³)-C(sp³) bonds by Palladium Catalyzed Cross-coupling of α -Diazoketones and Allylboronic Acids. *Org. Lett.* **2016**, *18*, 2503-2506. (Highlighted in *Synfacts* **2016**, *12*, 0845)
131. W. Yuan, L. Eriksson, K. J. Szabó*: Rhodium-Catalyzed Geminal Oxyfluorination and Oxytrifluoro-methylation of Diazocarbonyl Compounds. *Angew. Chem. Int. Ed.* **2016**, *55*, 8410-8415.
130. N. Miralles, R. Alam, K. J. Szabó*, E. Fernández*: Transition-Metal-Free Borylation of Allylic and Propargylic Alcohols. *Angew. Chem. Int. Ed.* **2016**, *55*, 4303-4307.
129. N. O. Ilchenko, M. A. Cortés, K. J. Szabó*: Palladium Catalyzed Iodofluorination of Alkenes using Fluoro-Iodoxole Reagent. *ACS Catal.* **2016**, *6*, 447-450.
128. Y. Yang, K. J. Szabó*: Synthesis of Allenes by Catalytic Coupling of Propargyl Carbonates with Aryl Iodides in the Presence of Diboron Species. *J. Org. Chem.* **2016**, *81*, 250-255.
127. Y. Zhao, K. J. Szabó*: Catalytic Borylative Opening of Propargyl Cyclopropane, Epoxide, Aziridine and Oxetane Substrates. Ligand Controlled Synthesis of Allenyl Boronates and Alkenyl Diboronates. *Angew. Chem. Int. Ed.* **2016**, *55*, 1502-1506.
126. A. Das, D. Wang, M.-C. Belhomme, K. J. Szabó*, *Org. Lett.* **2015**, *17*, 4754-4757. *ACS Editors' Choice* 9/16/15
125. R. Alam, T. Vollgraff, L. Eriksson, K. J. Szabó*: Synthesis of Adjacent Quaternary Stereocenters by Catalytic Asymmetric Allylboration. *J. Am. Chem. Soc.* **2015**, *137*, 11262-11265.
124. S. Agasti, S. Maity, K. J. Szabó*, K. J. D. Maiti*, Palladium-Catalyzed Synthesis of 2,3-Disubstituted Benzofurans: An Approach Towards the Synthesis of Deuterium Labeled Compounds. *Adv. Synth. Catal.* **2015**, *357*, 2331-2338.

123. W. Yuan, K. J. Szabó*: Catalytic Intramolecular Aminofluorination, Oxyfluorination, and Carbofluorination with a Stable and Versatile Hypervalent Fluoroiodine Reagent. *Angew. Chem. Int. Ed.* **2015**, *15*, 8533-8537.
122. T. S. N. Zhao, J. Zhao, K. J. Szabó*: Stereoselective Synthesis of 1,4-Diols by a Tandem Allylboration–Allenylboration Sequence. *Org. Lett.* **2015**, *17*, 2290-2293.
121. H.-P. Deng, D. Wang, K. J. Szabó*: Direct Allylation of Quinones with Allylboronates. *J. Org. Chem.* **2015**, *80*, 3343-3348.
120. P. G. Janson, N. O. Ilchenko, A. Diez-Varga, K. J. Szabó*: Effects of B₂pin₂ and PCy₃ on Copper Catalyzed Trifluoromethylation of Substituted Alkenes and Alkynes with the Togni Reagent. *Tetrahedron*, **2015**, *71*, 922-931.
119. N. O. Ilchenko, B. O. A. Tasch, K. J. Szabó*: Mild Silver Mediated Geminal Difluorination of Styrenes by Air and Moisture Stable Fluoroiodane Reagent. *Angew. Chem. Int. Ed.* **2014**, *53*, 12897-12901.
118. *Pincer and Pincer-Type Complexes: Applications in Organic Synthesis and Catalysis*. Eds. K. J. Szabó, O. Wendt. VCH-Wiley, [Weinheim 2014, ISBN: 978-3-527-33442-1](#). [\[summary\]](#)
117. A. Das, R. Alam, L. Eriksson, K. J. Szabó*: Stereocontrol in Synthesis of Homoallylic Amines. Syn Selective Direct Allylation of Hydrazones with Allylboronic Acids *Org. Lett.* **2014**, *16*, 3808-3811.
116. H.-P. Deng, L. Eriksson, K. J. Szabo*: Allylic sp³ C-H Borylation of Alkenes via Allyl-Pd intermediates. An Efficient Route to Allylboronates *Chem. Comm.* **2014**, *50*, 9207-9210.
115. T. S. N. Zhao, Y. Yang, T. Lessing, K. J. Szabó*: Borylation of Propargylic Substrates by Bimetallic Catalysis. Synthesis of Allenyl, Propargylic and Butadienyl Bpin Derivatives. *J. Am. Chem. Soc.* **2014**, *136*, 7563-7566. (Highlighted in *Synfacts*, **2014**, *10*, 0969).
114. R. Alam, A. Das, G. Huang, L. Eriksson, F. Himo, K. J. Szabó*: Stereoselective Allylboration of Imines and Indoles under Mild Conditions. In Situ E/Z Isomerization of Imines by Allylboroxines. *Chem. Sci.* **2014**, *5*, 2732-2738.
113. N. O. Ilchenko, P. G. Janson, K. J. Szabó*: Copper-Mediated Cyanotrifluoromethylation of Styrenes Using the Togni Reagent. *J. Org. Chem.* **2013**, *78*, 11087-11091. (Highlighted in *Synfacts*, **2014**, *10*, 191).
112. K. J. Szabó*: *Boron Mediated Multicomponent Reactions. In Science of Synthesis Reference Library: Multicomponent Reactions 2*. Ed T. J. J. Müller, **2013**, Thieme, Stuttgart pp 345-376.
111. B. Martín-Matute, K. J. Szabó, T. N. Mitchell: *Organotin Reagents in Cross Coupling. In Metal Catalyzed Cross-Coupling Reactions and More*. Eds. A. De Meijre, S. Bräse, M. Oestreich. **2014**, Wiley, Weinheim.

110. J. M. Larsson, S. R. Pathipati, K. J. Szabó*: Regio- and Stereoselective Allylic Trifluoromethylation and Fluorination using CuCF_3 and CuF Reagents. *J. Org. Chem.* **2013**, *78*, 7330-7336.
109. N. O. Ilchenko, P. G. Janson, K. J. Szabó*: Copper-mediated C–H Trifluoromethylation of Quinones. *Chem. Commun.* **2013**, *49*, 6614-6616. (Highlighted in *Synfacts*, **2013**, *9*, 998).
108. R. Alam, M. Raducan, L. Eriksson, K. J. Szabó*: Selective Formation of Adjacent Stereocenters by Allylboration of Ketones under Mild Neutral Conditions. *Org. Lett.* **2013**, *15*, 2546-2549.
107. J. M. Larsson, K. J. Szabó*: A Mechanistic Investigation of the Palladium-Catalyzed Synthesis of Allylic Silanes and Boronates from Allylic Alcohols. *J. Am. Chem. Soc.* **2013**, *135*, 443-455.
106. M. Raducan, R. Alam, K. J. Szabó*: Palladium-Catalysed Synthesis and Isolation of Functionalized Allylboronic Acids. Selective, Direct Allylboration of Ketones. *Angew. Chem. Int. Ed.* **2012**, *51*, 13050-13053. (Highlighted in *Synfacts*, **2013**, *issue 3*, 314).
105. T. S. N. Zhao, K. J. Szabó*: Trifluoromethylation of Propargylic Halides and Trifluoroacetates Using $(\text{Ph}_3\text{P})_3\text{Cu}(\text{CF}_3)$. *Org. Lett.* **2012**, *14*, 3966-3969. (Highlighted in *Synfacts* **2012**, *issue 11*, 1251).
104. P. G. Janson, I. Ghoneim, N. O. Ilchenko, K. J. Szabó: Electrophilic Trifluoromethylation by Copper-Catalyzed Addition of CF_3 -Transfer Reagents to Alkenes and Alkynes. *Org. Lett.* **2012**, *14*, 2882-2885.
103. R. Alam, L. T. Pilarski, E. Pershagen, K. J. Szabó*: Stereoselective Intermolecular Allylic C-H Trifluoroacetoxylation of Functionalized Alkenes. *J. Am. Chem. Soc.* **2012**, *134*, 8778-8781.
102. K. J. Szabó*: *C-B and C-Si Bond Forming Reactions by C-H Functionalization*. In *Science of Synthesis Reference Library : Cross-Coupling and Heck-Type Reactions 2*. Ed. J. P. Wolfe, **2013**, Thieme, Stuttgart pp 485-522.
101. K. J. Szabó*: Pincer Complexes as Catalysts in Organic Chemistry. *Topics in Organometallic Chemistry Vol 40; Organometallic Pincer Chemistry*, Eds: G. v. Koten and D. Millstein, **2012**, 203-242.
100. L. T. Pilarski, K. J. Szabó*: Palladium-Catalyzed Direct Synthesis of Organoboronic acids. *Angew. Chem. Int. Ed.* **2011**, *50*, 8230-8232.
99. J. M. Larsson, T. S. N. Zhao, K. J. Szabó*: Palladium-catalyzed Oxidative Allylic C-H Silylation. *Org. Lett.* **2011**, *13*, 1888-1891.
98. L. T. Pilarski, K. J. Szabó*: Diphenyliodonium hexafluorophosphate, In *Electronic Encyclopedia of Reagents for Organic Synthesis*, Eds: L. A. Paquette, P. Fuchs, D. Crich, G. A. Molander, DOI: 10.1002/047084289X.rm01349.

97. L. T. Pilarski, P. G. Janson, K. J. Szabó*: Palladium-Catalyzed Selective Acyloxylation Using Sodium Perborate as Oxidant. [*J. Org. Chem.* **2011**, *76*, 1503-1506.](#)
96. N. Selander, J. R. Paasch, K. J. Szabó*: Palladium-Catalyzed Allylic C–OH Functionalization for Efficient Synthesis of Functionalized Allylsilanes. [*J. Am. Chem. Soc.* **2011**, *133*, 409-411.](#) (Highlighted in *Synfacts* **2011**, issue 4, 434)
95. N. Selander, K. J. Szabó*: Catalysis by Palladium Pincer Complexes. In special issue “Frontiers in Transition Metal Catalyzed Reactions”. [*Chem. Rev.* **2011**, *111*, 2048-2076.](#)
94. L. T. Pilarski, K. J. Szabó*: Palladium Pincer Complex Catalyzed Functionalization of Electrophiles. *Curr. Org. Chem.* **2011**, *15*, 3389-3414.
93. N. Selander, B. Willy, K. J. Szabó*: Selective C-H Borylation of Alkenes by Palladium Pincer Complex Catalyzed Oxidative Functionalization. [*Angew. Chem. Int. Ed.* **2010**, 4051-4053.](#)
92. K. J. Szabó*: Mechanism of the Oxidative Addition of Hypervalent Iodonium Salts to Palladium(II) Pincer-Complexes. [*J. Mol. Cat. A* **2010**, *324*, 56-63.](#)
91. L. T. Pilarski, N. Selander, D. Böse, K. J. Szabó*: Catalytic Allylic C-H Acetoxylation and Benzoyloxylation via Suggested (η^3 -Allyl)palladium(IV) Intermediates. [*Org. Lett.* **2009**, *11*, 5518-5521.](#)
90. V. J. Olsson, K. J. Szabó*: Functionalization of Unactivated Alkenes through Iridium-Catalyzed Borylation of Carbon-Hydrogen Bonds. Mechanism and Synthetic Applications. [*J. Org. Chem.* **2009**, *74*, 7715-7723.](#)
89. N. Selander, K. J. Szabó: Performance of SCS Palladium Pincer-Complexes in Borylation of Allylic Alcohols. Control of the Regioselectivity in the One-Pot Borylation-Allylation Process. [*J. Org. Chem.* **2009**, *74*, 5695-5698.](#)
88. J. Aydin, J. M. Larsson, N. Selander, K. J. Szabó*: Pincer Complex-Catalyzed Redox Coupling of Alkenes with Iodonium Salts via Presumed Palladium(IV) Intermediates. [*Org. Lett.* **2009**, *11*, 2852-2854.](#)
87. N. Selander, K. J. Szabó*: Synthesis and Transformation of Organoboronates and Organostannanes by Pincer-Complexes. [*Dalton Transactions*, **2009**, 6267-6279.](#)
86. N. Selander, K. J. Szabó*: [2,6-Bis[(phenylseleno- κ Se)methyl]phenyl- κ C]chloropalladium, In Electronic Encyclopedia of Reagents for Organic Synthesis, Eds: L. A. Paquette, P. Fuchs, D. Crich, G. A. Molander, Wiley, Chichester, **2009**. DOI: 10.1002/047084289X.rm01104
85. M. Seenivasaperumal, H.-J. Federsel, K. J. Szabó*: Mechanism of the Asymmetric Sulfoxidation in the Esomeprazole Process. Effects of the Imidazole Backbone for the Enantioselection. [*Adv. Synth. Catal.* **2009**, *351*, 903.](#)
84. J. Aydin, C. S. Conrad, K. J. Szabó*: Stereoselective Pincer-Complex Catalyzed C-H Functionalization of Benzyl Nitriles under Mild Conditions. An Efficient Route to β -Aminonitriles. [*Org. Lett.* **2008**, *10*, 5175-5178.](#) (Highlighted in *Synfacts* **2009**, issue 2, 166)

83. J. Aydin, A. Rydén, K. J. Szabó*: Chiral palladium pincer-complex catalyzed asymmetric condensation of sulfonimines and isocyanoacetate. [*Tetrahedron: Asymmetry* **2008**, *19*, 1867-1870.](#)
82. N. Selander, K. J. Szabó*: Synthesis of Stereodefined Substituted Cycloalkenes by a One-Pot Catalytic Boronation Allylation Metathesis Sequence. [*Adv. Synth. Catal.* **2008**, *350*, 2045-2051.](#)
81. V. J. Olsson, K. J. Szabó*: Regio- and Stereoselective Synthesis of Allylsilanes and Siladienes by a One-Pot Catalytic C-H Borylation - Suzuki-Miyaura Coupling Sequence. [*Org. Lett.* **2008**, *10*, 3129.](#)
80. G. Dutheuil, N. Selander, K. J. Szabó*, V. K. Aggarwal*: Direct Synthesis of Functionalized Allylic Boronic Esters from Allylic Alcohols and Inexpensive Reagents and Catalysts. [*Synthesis*, **2008**, 2293-2297.](#)
79. N. Selander, K. J. Szabó*: Single-Pot Transformations Based on Coupling of Catalytically Generated Allyl Boronates with *in situ* Hydrolyzed Acetals. [*Chem. Commun.* **2008**, 3420-3422.](#)
78. J. Aydin, K. J. Szabó: Palladium Pincer-Complex Catalyzed C-C Coupling of Allyl Nitriles with Tosyl-Imines via Regioselective Allylic C-H Bond Functionalization. [*Org. Lett.* **2008**, *10*, 2881-2884.](#)
77. N. Selander, K. J. Szabó*: Efficient Synthesis of α -Amino Acids via Organoboronate Reagents. In "*Current Frontiers in Asymmetric Synthesis and Application of alpha-Amino Acids.*" ACS Symposium Series 1009.. Eds: V. A. Soloshonok and K. Izawa, Oxford University Press, **2009**.
76. M. Gagliardo, N. Selander, N. C. Mehendale, G. van Koten, R. J. M. Klein Gebbin,* K. J. Szabó*: Catalytic Performance of Symmetrical and Unsymmetrical Sulfur Containing Pincer Complexes. Synthesis and Tandem Catalytic Activity of the First PCS-Pincer Palladium Complex. [*Chem. Eur. J.* **2008**, *14*, 4800-4809.](#)
75. N. Selander, A. Kipke, S. Sebelius, K. J. Szabó*: Petasis Borono-Mannich Reaction and Allylation of Carbonyl Compounds via Transient Allyl Boronates Generated by Palladium Catalyzed Substitution of Allyl Alcohols. An Efficient One-Pot Route to Stereodefined α -Amino Acids and Homoallyl Alcohols. [*J. Am. Chem. Soc.* **2007**, *129*, 13723-13731.](#) (Highlighted in *Synfacts* **2008**, issue 2, 189)
74. V. J. Olsson, K. J. Szabó*: Selective One-Pot Carbon-Carbon Bond Formation by Catalytic Boronation of Unactivated Cycloalkenes and Subsequent Coupling. [*Angew. Chem. Int. Ed.* **2007**, *46*, 6891-6893.](#)
73. J. Aydin, K. SentilKumar, L. Eriksson, K. J. Szabó*: Palladium Pincer Complex Catalyzed Condensation of Sulfonimines and Isocyanoacetate to Imidazoline Derivatives. Dependence of the Stereoselectivity on the Ligand Effects. [*Adv. Synth. Catal.* **2007**, *349*, 2585-2594.](#)
72. A. Träff, G. N. Nilsson, K. J. Szabó*, L. Eriksson*: Application of Iridium Pincer Complexes in Hydrogen Isotope Exchange Reactions. [*J. Organomet. Chem.* **2007**, *692*, 5529-5531.](#)

71. K. J. Szabó*: Synthesis and Transformation of Allyl- and Allenyl-metal Species by Pincer Complex Catalysis. In *The Chemistry of Pincer Compounds*, Eds D. Morales-Morales and C. Jensen, Elsevier, Chapter 2, **2007**, 26-43.
70. J. Aydin, K. SenthilKumar, M. J. Sayah, O. A. Wallner, K. J. Szabó: Synthesis and Catalytic Application of Chiral BINOL and Biphenanthrol Based Pincer Complexes. Selective Allylation of Sulfonimines with Allyl Stannane and Allyl Trifluoroborate. [*J. Org. Chem.* **2007**, *72*, 4689-4697.](#) (Highlighted in *Synfacts* **2007**, issue 9, 954)
69. M. Seenivasaperumal, H.-J. Federsel, A. Ertan, K. J. Szabó*: Factors Influencing the Selectivity in Asymmetric Oxidation of Sulfides Attached to Nitrogen Containing Heterocycles. [*Chem. Commun.* **2007**, 2187 – 2189.](#)
68. N. Selander, S. Sebelius, C. Estay, K. J. Szabó*: Highly Selective and Robust Palladium-Catalyzed Carbon-Carbon Coupling between Allyl Alcohols and Aldehydes via Transient Allylboronic Acids. [*Eur. J. Org. Chem.* **2006**, 4085-4087.](#)
67. S. Sebelius, V. J. Olsson, O. A. Wallner, K. J. Szabó*: Palladium-Catalyzed Coupling of Allylboronic Acids with Iodobenzenes. Selective Formation of the Branched Allylic Product in the Absence of Directing Groups. [*J. Am. Chem. Soc.* **2006**, *128*, 8150-8151.](#) (Highlighted in *Synfacts* **2006**, issue 9, 939)
66. J. Aydin, N. Selander, K. J. Szabó*: Strategies for Fine-Tuning the Catalytic Activity of Pincer-Complexes. [*Tetrahedron Lett.* **2006**, *47*, 8999-9001.](#)
65. O. A. Wallner, K. J. Szabó*: Potassium Trifluoro-2-Propenylborate, Electronic Encyclopedia of Reagents for Organic Synthesis, Ed: L. A. Paquette, Wiley, Chichester, **2006**. DOI: 10.1002/047084289X.rn00710.
64. J. Kjellgren, M. Kritikos, K. J. Szabó*: Synthesis and Structural Features of α -Acyloxy-(η^3 -allyl)palladium Complexes. [*J. Organomet. Chem.* **2006** *691*, 3640-3645.](#)
63. O. A. Wallner, K. J. Szabó*: Regio- and Stereoselective Palladium Pincer-Complex Catalyzed Allylation of Sulfonimines with Trifluoro(allyl)borates and Allyl Stannanes. A Combined Experimental and Theoretical Study. [*Chem. Eur. J.* **2006**, *12*, 6976-6983.](#)
62. V. J. Olsson, S. Sebelius, N. Selander, K. J. Szabó*: Direct Boronation of Allyl Alcohols with Diboronic Acid using Palladium Pincer-Complex Catalysis. A Remarkably Facile Allylic Displacement of the Hydroxy Group Under Mild Reaction Conditions. [*J. Am. Chem. Soc.* **2006**, *128*, 4588-4589.](#)
61. K. J. Szabó*: Palladium-Pincer-Complex-Catalyzed Transformations Involving Organometallic Species. [*Synlett* **2006**, 811-824.](#)
60. O. A. Wallner, K. J. Szabó*: Employment of Pincer-Complexes in Phenylselenation of Organohalides. [*J. Org. Chem.* **2005**, *70*, 9215-9221.](#)
59. S. Sebelius, Vilhelm J. Olsson, K. J. Szabó*: Palladium Pincer Complex Catalyzed Substitution of Vinyl Cyclopropanes, Vinyl Aziridines, and Allyl Acetates with

Tetrahydroxydiboron. An Efficient Route to Allylboronic Acids and Potassium Trifluoro(allyl)borates. [*J. Am. Chem. Soc.* **2005**, *127*, 10478-10479.](#)

58. O. A. Wallner, V. J. Olsson, L. Eriksson, K. J. Szabó*: Synthesis of New Chiral Pincer-complex Catalysts for Asymmetric Allylation of Sulfonimines. [*Inorg. Chim. Acta* **2006**, *359*, 1767-1772.](#)

57. J. Kjellgren, J. Aydin, O. A. Wallner, I. V. Saltanova, K. J. Szabó*: Palladium Pincer-Complex Catalyzed Cross-Coupling of Vinyl Epoxides and Aziridines with Organoboronic Acids. [*Chem. Eur. J.* **2005**, *11*, 5260-5268.](#)

56. S. Sebelius, K. J. Szabó*: Allylation of Aldehyde and Imine Substrates with in Situ Generated Allylboronates. A Simple Route to Enantioenriched Homoallyl Alcohols. [*Eur. J. Org. Chem.* **2005**, 2539-2547.](#)

55. N. Solin, O. A. Wallner, K. J. Szabó: Palladium Pincer Complex-Catalyzed Allylation of Tosylimines by Potassium Trifluoro(allyl)borates. [*Org. Lett.* **2005**, *7*, 689-691.](#)

54. J. Kjellgren, H. Sundén, K. J. Szabó*: Palladium Pincer Complex-Catalyzed Stannyl and Silyl Transfer to Propargylic Substrates. Synthetic Scope and Mechanism. [*J. Am. Chem. Soc.* **2005**, *127*, 1787-1796.](#)

53. O. A. Wallner, K. J. Szabó*: Palladium Pincer-Complex Catalyzed Allylic Stannylation with Hexaalkylditin Reagents. [*Org. Lett.* **2004**, *6*, 1829-1831.](#)

52. K. J. Szabó*: Palladium-Catalyzed Electrophilic Allylation Reactions via Bis-Allylpalladium Complexes and Related Intermediates. [*Chem. Eur. J.* **2004**, *10*, 5268-5275.](#)

51. N. Solin, J. Kjellgren, K. J. Szabó*: Pincer Complex Catalyzed Allylation of Aldehyde and Imine Substrates via Nucleophilic η^1 -Allylpalladium Intermediates. A New Concept for Palladium Catalyzed Allylic Substitution Reactions. [*J. Am. Chem. Soc.* **2004**, *126*, 7026-7033.](#)

50. J. Kjellgren, H. Sundén, K. J. Szabó*: Palladium Pincer Complex-Catalyzed Trimethyltin Substitution of Functionalized Propargylic Substrates. An Efficient Route to Propargyl- and Allenyl-Stannanes [*J. Am. Chem. Soc.* **2004**, *126*, 474-475.](#)

49. S. Sebelius, O. A. Wallner, K. J. Szabó*: Palladium-Catalyzed Coupling of Allyl Acetates with Aldehyde and Imine Electrophiles in the Presence of Bis(pinacolato)diboron [*Org. Lett.* **2003**, *5*, 3065-3068.](#)

48. N. Solin, J. Kjellgren, K. J. Szabó*: Palladium-catalyzed Electrophilic Substitution via Mono-allylpalladium Intermediates [*Angew. Chem. Int. Ed.* **2003**, *42*, 3656-3658.](#)

47. O. A. Wallner, K. J. Szabó*: Origin of the Stereoselectivity in Palladium-catalyzed Electrophilic Substitution via Bis-allylpalladium Complexes [*Chem. Eur. J.* **2003**, *9*, 4025-4030.](#)

46. O. A. Wallner, K. J. Szabó*: Palladium-catalyzed Electrophilic Substitution of Allyl Chlorides and Acetates via Bis-allylpalladium Intermediates [*J. Org. Chem.* **2003**, *68*, 2934-2943.](#)

45. O. A. Wallner, K. J. Szabó*: Regioselective Palladium-Catalyzed Electrophilic Allylic Substitution in the Presence of Hexamethylditin [*Org. Lett.* **2002**, *4*, 1563-1566.](#)
44. E. Hupe, P. Knochel, K. J. Szabó*: Mechanism of the Stereoselective Alkyl Group Exchange Between Alkyl-Boranes and Alkyl-Zinc Compounds. Quest for Novel Types of Boron-Metal Exchange Reactions. [*Organometallics* **2002**, *21*, 2203-2207.](#)
43. J. Kjellgren, K. J. Szabó*: Synthesis of Stereodefined Vinyl-Tetrahydropyran and Vinyl-octahydrochromene Derivatives via Acetalization-cyclization of Allylsilanes with Aldehydes. Origin of the High Stereoselectivity. [*Tetrahedron Lett.* **2002**, *43*, 1123-1126.](#)
42. N. Solin, K. J. Szabó*: Mechanism of the η^3 - η^1 - η^3 Isomerization in Allylpalladium Complexes: Solvent Coordination, Ligand and Substituent Effects. [*Organometallics* **2001**, *20*, 5464-5471.](#)
41. I. Macsári, K. J. Szabó*: Palladium Catalyzed Cyclization of Allylsilanes with Nucleophilic Displacement of the Silyl Functionality. [*Chem. Eur. J.* **2001**, *7*, 4097-4106.](#)
40. N. Solin, S. Narayan, K. J. Szabó*: Palladium-Catalyzed Tandem Bis-allylation of Isocyanates. [*Org. Lett.* **2001**, *3*, 909-912.](#)
39. N. Solin, S. Narayan, K. J. Szabó*: Control of the Regioselectivity in Catalytic Transformations Involving Amphiphilic Bis-Allylpalladium Intermediates: Mechanism and Synthetic Applications. [*J. Org. Chem.* **2001**, *66*, 1686-1693.](#)
38. K. J. Szabó*: Nature of the Interaction between β -Substituents and the Allyl Moiety in (η^3 -Allyl)palladium Complexes. [*Chem. Soc. Rev.*, **2001**, *30*, 136-143.](#)
37. K. J. Szabó*: Umpolung of the Allyl-palladium Reactivity. Mechanism and Regioselectivity of the Electrophilic Attack on Bis-Allylpalladium Complexes Formed in Palladium Catalyzed Transformations. [*Chem. Eur. J.* **2000**, *6*, 4413-4421.](#)
36. I. Macsári, K. J. Szabó*: Umpolung the Reactivity of Allylsilanes. Palladium(II) Catalyzed Cyclization of Allylsilyl Alcohols: A New Route to Substituted 2-Vinyltetrahydrofurans. [*Tetrahedron Lett.* **2000**, *41*, 1119-1122.](#)
35. I. Macsári, E. Hupe, K. J. Szabó*: Regioselective Catalytic Transformations Involving β -Substituted (η^3 -Allyl)palladium Complexes: An Efficient Route to Functionalized Allylsilanes. [*J. Org. Chem.* **1999**, *64*, 9547-9556.](#)
34. C. Jonasson, M. Kritikos, J.-E. Bäckvall*, K. J. Szabó*: Asymmetric Allyl-metal Bonding in Substituted (η^3 -Allyl)palladium Complexes: X-ray Structures of *cis* and *trans*-4-acetoxy- $[\eta^3$ -(1,2,3)-cyclohexenyl]palladium Chloride Dimers. [*Chem. Eur. J.* **2000**, *6*, 432-436.](#)
33. I. Macsári, K. J. Szabó*: Nature of the Interactions between the β -Silyl Substituent and Allyl Moiety in (η^3 -Allyl)palladium Complexes. A Combined Experimental and Theoretical Study. [*Organometallics* **1999**, *18*, 701-708.](#)
32. I. Macsári, K. J. Szabó*: Copper(II) Mediated Regioselective Acetoxylation of Allylic Acetates and 1,4-Diacetoxylation of Alkenes. [*Tetrahedron Lett.* **1998**, *39*, 6345-6348.](#)

31. A. Aranyos, G. Csajnyik, K. J. Szabó*, J.-E. Bäckvall*: Evidence for a Ruthenium Dihydride Species as the Active Catalyst in the RuCl₂(PPh₃)₃-Catalyzed Hydrogen Transfer Reaction in the Presence of Base, [*Chem. Commun.* **1999**, 351-352.](#)
30. K. J. Szabó*: Benzoquinone-Induced Stereoselective Chloride Migration in (η^3 -allyl)palladium Complexes. A Theoretical Mechanistic Study Complemented by Experimental Verification. [*Organometallics*, **1998**, *17*, 1677-1686.](#)
29. K. J. Szabó,* H. Frisell, L. Engman,* M. Piatek, B. Oleksyn, J. Sliwinski: α -(Phenylselenyl) Ketones –Structure, Molecular Modelling and Rationalization of their Glutathione Peroxidase-like Activity, [*J. Mol. Struct.* **1998**, *448*, 21-28.](#)
28. E. Hupe, K. Itami, A. Aranyos, K. J. Szabó*, J.-E. Bäckvall*: Unsymmetrical Functionalization of 1,3-Cyclohexadienes: Palladium-Catalyzed Stereoselective 1,4-Acyloxy-Alkoxylation, [*Tetrahedron* **1998**, *54*, 5375-5384.](#)
27. A. Aranyos, K. J. Szabó, J.-E. Bäckvall*: Palladium-Catalyzed 1,4-Acetoxy-Trifluoroacetoxylation of Cyclic 1,3-Dienes. Scope and Mechanism, [*J. Org. Chem.* **1998**, *63*, 2523-2529.](#)
26. K. J. Szabó: Effects of Polar γ -Substituents on the Structure and Stability of Palladacyclobutane Complexes, [*J. Mol. Struct.Theochem* **1998**, *455*, 205-211.](#)
25. K. J. Szabó,* E. Hupe, A. Larsson: Stereoelectronic Control on the Kinetic Stability of β -Acetoxy Substituted (η^3 -Allyl)palladium Complexes in a Mild Acidic Medium, [*Organometallics* **1997**, *16*, 3779.](#)
24. K. J. Szabó*: Nature of the Interactions between Polar β -Substituents and Palladium in (η^3 -Allyl)palladium Complexes. A Combined Experimental and Theoretical Study, [*Chem. Eur. J.* **1997**, *3*, 592-600.](#)
23. K. J. Szabó*: Effects of β -Substituents and Ancillary Ligands on the Structure and Stability of (η^3 -Allyl)palladium Complexes. Implications for the Regioselectivity in Nucleophilic Addition Reactions, [*J. Am. Chem. Soc.* **1996**, *118*, 7818-7826.](#)
22. A. Aranyos, K. J. Szabó, J.-E. Bäckvall*, A. N. Castano: Central versus Terminal Attack in Nucleophilic Addition to (η^3 -Allyl)palladium Complexes. Ligand Effects and Mechanism, [*Organometallics* **1997**, *16*, 1058-1064.](#)
21. C.-H. Ottoson, K. J. Szabó, D. Cremer*: Tris-9-borabicyclo[3.3.1]nonyl Silylium Cation: A Weakly Coordinated Silylium Cation in Solution, [*Organometallics* **1997**, *16*, 2377.](#)
20. K. J. Szabó*: Effects of the Ancillary Ligands on Palladium Carbon Bonding in (η^3 -Allyl)palladium Complexes. Implications for Nucleophilic Attack at the Allylic Carbons, [*Organometallics* **1996**, *15*, 1128-1133.](#)

19. A. N. Castano, A. Aranyos, K. J. Szabó, J.-E. Bäckvall*: Nucleophilic Attack on (π -Allyl)palladium Complexes: Direction of the Attack to the Central or Terminal Carbon Atom by Ligand Control, *Angew. Chem. Int. Ed. Engl.* **1995**, *34*, 2551-2553.
18. K. J. Szabó, E. Kraka, D. Cremer: Trishomocyclopropylium Cations - Structure, Stability, Conformation, Charge Distribution, Magnetic Properties, and Rearrangement Possibilities *J. Org. Chem.* **1996**, *61*, 2783-2800.
17. D. Cremer,* E. Kraka, K. J. Szabó: General and Theoretical Aspects of the Cyclopropyl Group "Chemistry of Functional Groups. Vol. 2 The Chemistry of the Cyclopropyl Group." John Wiley and Sons, Chichester, **1995**, 43-137.
16. K. J. Szabó, D. Cremer*: A Route to a Kinetically Stabilised Protonated Spirocyclopentane with a Pentacoordinated Carbon Atom - The Missing Link between Bicyclo[3.2.0]hept-3-yl and 7-Norbornyl Cation *J. Org. Chem.* **1995**, *60*, 2257-2259.
15. D. Cremer, K. J. Szabó*: Ab Initio Studies of Six-Membered Rings, Present Status and Future Developments. "Conformational Behavior of Six-Membered Rings; Analysis, Dynamics, and Stereoelectronic Effects", VCH, **1995**, 59-134.
14. K. J. Szabó, S. Gronowitz*: Direct Bromination of Dithieno[3,2-b:3',2'-d]pyridine *J. Heterocyclic Chem.* **1993**, *30*, 561-2.
13. K. J. Szabó, S. Gronowitz*: Nitration of Dithieno[3,2-b:3',2'-d]pyridine *J. Heterocyclic Chem.* **1993**, *30*, 543-4.
12. K. J. Szabó, A.-B. Hörnfeldt, S. Gronowitz*: ^{15}N -CIDNP Measurements and Ab Initio Calculations on the Nitration of Dithieno[3,4-b:3',4'-d]pyridine *N*-oxide *J. Chem. Soc. Perkin Trans. II* **1992**, 1875.
11. S. Gronowitz,* K.J. Szabó, T. Olugbade: Orientation Effects in the Nitration of Dithieno[b,d]pyridine *N*-oxides. Its Dependence on the Acidity of the Reaction Medium. *J. Heterocyclic Chem.* **1992**, *29*, 1635-1640.
10. K. J. Szabó,* A.-B. Hörnfeldt, S. Gronowitz: Theoretical Study on Mechanism and Selectivity of Electrophilic Aromatic Nitration. *J. Am. Chem. Soc.* **1992**, *114*, 6827-683.
9. S. Gronowitz*, K.J. Szabó, M.A. Hassan: Experimental and Theoretical Study of the Orientation in Lithiation of Dithieno[2,3-b:3',2'-d]pyridine. *J. Org. Chem.* **1992**, *57*, 4552-4555.
8. K. J. Szabó, A.-B. Hörnfeldt, S. Gronowitz*: Theoretical Study of Orientation in the Nitration of Dithieno[2,3-b:3',2'-d]pyridine. *J. Mol. Struct. Theochem.* **1992**, *258*, 67-82.
7. K. J. Szabó, A.-B. Hörnfeldt: Theoretical Study on the Nitration of Pyridine: Comparison with Electrophilic Substitution of Dithieno[3,4-b:3',4'-d]pyridine. *J. Mol. Struct. Theochem.* **1992**, *258*, 53-65.

6. K. J. Szabó, S. Gronowitz,* A.-B. Hörnfeldt: Experimental and Theoretical Study of Orientation in the Nitration of Dithieno[3,4-b:3',4'-d]pyridine. [*J. Org. Chem.* **1991**, *56*, 1590-96.](#)
5. S. Gronowitz,* K. J. Szabó, J. O. Oluwadiya: Nitration of Dithieno[3,4-b:3',2'-d]pyridine. *J. Heterocyclic Chem.* **1991**, *28*, 351-2.
4. K.J. Szabó, G. Timári, S. Gronowitz*: Regioselectivity of Nitration of Thieno-fused Quinoline and Isoquinoline Derivatives. *Chemica Scripta* **1989**, *29*, 313-314.
3. K. J. Szabó, J. Császár*: Investigation of Heteroaromatic Nucleophilic Substitution Reaction. [*J. Mol. Struct. Theochem* **1990**, *204*, 45-56.](#)
2. K. J. Szabó, J. Császár*, A. Toró: Synthesis of New Heterocyclic Ring Systems via Nucleophilic Substitution of Pyrimido[4,5-d]pyridazines. [*Tetrahedron*, **1989**, *45*, 4485-96.](#)
1. K. J. Szabó*: Structures of Sigma Complexes in Nitration Reactions of Monosubstituted Benzene Derivatives. [*J. Mol. Struct. Theochem* **1988**, *181*, 1-9.](#)