

Richard M.W. Wong's Research Publication

[International Journal Articles](#)

163. "Roles of Electrostatic Interaction and Dispersion in CH \cdots CH, C-H \cdots π and $\pi\cdots\pi$ in Dimers", Y. Cao and M.W. Wong, *ChemPhysChem.*, submitted.
162. "Experimental Upfield Chemical Shift as Reliable Indicator for Remarkably Aromatic Aza[13]annulenes and Unique Hydrogen-Bonding Between Methyl Protons and an Ester Function", Y. Ting, M.W. Wong and Y. H. Lai. *J. Org. Chem.*, submitted.
161. "Crystal Packing Induced Domino Effect of Isomerisation - An Oxygen-Initiated Diradical Chain Mechanism", A. Chanthapally, H. Yang, H.S. Quah, R.D. Webster, M.W. Wong, and J.J. Vittal, *J. Am. Chem. Soc.*, submitted.
160. "Oxyanion Hole Stabilization by CH \cdots O Interaction in a Transition State - A Three-Point Interaction Model for *Cinchona* Alkaloid-Catalyzed Asymmetric Methanolysis of *Meso*-Cyclic Anhydrides", H. Yang and M.W. Wong, *J. Am. Chem. Soc.* **135** (2013) 5808-5818.
159. "Anion Recognition by Azophenol-Thiourea Based Chromogenic Receptors: A Combined DFT and Molecular Dynamics Investigation", M.W. Wong, H. Xie and S.T. Kwa, *J. Mol. Mod.* **19** (2013) 205-213.
158. "Origin of Asymmetric Induction in Bicyclic Guanidine-Catalyzed Thio-Michael Reaction: A Bifunctional Mode of Lewis and Brønsted Acid Activations", B. Cho, C.-H. Tan, and M.W. Wong, *J. Org. Chem.* **77** (2012) 6553-6562.
157. "Selenium Blue-alpha and -beta: Turning on the fluorescence of a Pyrenyl Fluorophore via Oxidative Cleavage of the Se-C Bond by Reactive Oxygen Species", W. Chen, B. P. Bay, M.W. Wong, and D.J. Huang, *Tetrahedron Lett.* **253** (2012) 3843-384.
156. "Mechanistic Investigation on the Formation and Dehydrogenation of Calcium Amidoborane Ammoniate", Y.S. Chua, W. Li, W.J. Shaw, G.T. Wu, T. Autrey, Z. Xiong, M.W. Wong, and P. Chen, *ChemSusChem* **5** (2012) 927-931.
155. "(*S*)-Proline-Catalyzed Nitro-Michael Reactions: Towards a Better Understanding of the Catalytic Mechanism and Enantioselectivity", H. Yang and M.W. Wong, *Org. Biomol. Chem.* **10** (2012) 3229-3215.

154. "Computational Design of Thiourea-based Cyclophane Anion Sensors", H. Xie and M.W. Wong, *Aust. J. Chem.* **65** (2012) 303-313.
153. "Monoammoniate of Calcium Amidoborane: Synthesis, Structure, and Hydrogen-Storage Properties", Y.S. Chua, H. Wu, W. Zhou, T.J. Udovic, G.T. Wu, Z. Xiong, M.W. Wong, and P. Chen, *Inorg. Chem.* **51** (2012) 1599-1603.
152. " β -Amino Acid-Catalyzed Asymmetric Michael Additions: Design of Organocatalysts with Catalytic Acid/Base Dyad Inspired by Serine Proteases", H. Yang and M.W. Wong, *J. Org. Chem.* **76** (2011) 7399-7045.
151. " π -Complexed Polyfluoroarenes: A Reactivity, Bonding and Spectroscopic Study of $(\eta^6\text{-C}_6\text{F}_6)\text{Cr}(\eta^6\text{-C}_6\text{H}_6)$ and Related Molecules", M. J. McGlinchey and M.W. Wong, *New J. Chem.* **35** (2011) 2066-2073.
150. "Sequential Catalytic Role of Bifunctional Bicyclic Guanidine in Asymmetric Phospha-Michael Reaction", B. Cho, C.-H. Tan, and M.W. Wong, *Org. Biomol. Chem.* **9** (2011) 4550-4557.
149. "Synthesis, Structure and Dehydrogenation of Magnesium Amidoborane Monoammoniate", Y.S. Chua, G. Wu, Z. Xiong, A. Karkamkar, J. Guo, M. Jian, M.W. Wong, T. Autrey, and P. Chen, *Chem. Commun.* **46** (2010) 5752-5754.
148. "The Role Of Metal Cation in Electron-Induced Dissociation of Tryptophan", L. Feketeová, M.W. Wong and R. A. J. O'Hair, *Eur. Phys. J. D*, **60** (2010) 11-20.
147. "Direct Asymmetric Aldol Reactions between Aldehydes and Ketones Catalyzed by L-Tryptophan in the Presence of Water", Z. Jiang, H. Yang, X. Han, J. Luo, M.W. Wong and Y. Lu, *Org. Biomol. Chem.* **8** (2010) 1368-1377.
146. "Interaction of Ammonia Borane with Li_2NH and Li_3N ", Z. Xiong, Y. Chua, G. Wu, L. Wang, M.W. Wong, Z.M. Kam, T. Autrey, T. Kemmitt and P. Chen, *Dalton Trans.* **39** (2010) 720-722.
145. "Structure of 4,4-Bis(phenyl)-2,*N,N*-sulphonyl-dimethylbutylamine: Interplay of C-H \cdots N, C-H \cdots O=S, and $\pi\cdots\pi$ Interactions", Ran J. and M.W. Wong, *Aust. J. Chem.* **62** (2009) 1062-1067.
144. "Water Helicate, $(\text{H}_2\text{O})_7$ Hosted by Diamondoid Metal–Organic Framework", M.H. Mir, L. Wang, M.W. Wong and J.J. Vittal, *Chem. Commun.* (2009) 4539-4541.
143. "Synthesis of a Chiral Quaternary Carbon Center Bearing a Fluorine Atom: Enantioselective and Diastereoselective Guanidine-Catalyzed Addition of

- Fluorocarbon Nucleophiles", Z. Jiang, Y. Pan, Y. Zhao, T. Ma, R. Lee, Y. Yang, K.-W. Huang, M.W. Wong and C.-H. Tan, *Angew. Chem. Int. Ed.* **48** (2009) 3627-3631.
142. "Mechanism of Halogen-Catalyzed Mukaiyama Aldol Reactions: Concerted or Stepwise?", L. Wang and M.W. Wong, *Tetrahedron Lett.* **49** (2008) 3916-3920.
141. "Homolytic S-S Bond Dissociation of 11 Bis(thiocarbonyl)disulfides R-C(=S)-S-S-C(=S)R and Prediction of a Novel Rubber Vulcanization Accelerator", A.M. Mak, R. Steudel, and M.W. Wong, *Asian. J. Chem.* **3** (2008) 1026-1034.
140. "Complex formation of the Vulcanization Accelerator Tetramethyldiuram Disulfide (TMTD) and Related Molecules with Various Zinc Compounds Including Zinc Oxide Clusters (Zn₄O₄)", R. Steudel, Y. Steudel and M.W. Wong, *Chem. Eur. J.* **14** (2008) 919-932.
139. "Highly Diastereoselective and Enantioselective Direct Organocatalytic *Anti*-selective Mannich Reaction Employing *N*-tosylimines", L. Cheng, X. Han, H. Huang, M.W. Wong and Y. Lu, *Chem. Commun.* (2007) 4143-4145.
138. "Reaction of the Radical Pair NO₂[•] and CO₃^{•-} on 2-[6-(4'-Amino)phenoxy-3H-xanthen-3-on-9-yl]benzoic Acid (APF)", A.M. Mak, M. Whiteman and M.W. Wong, *J. Phys. Chem. A*, **111** (2007) 8202-8210.
137. "Carboxyketenes, Methyleneketenes, Vinylketenes, Oxetanediones, Ynols, and Ylidic Ketenes from Meldrum's Acid Derivatives", L. George, M.W. Wong and C. Wentrup, *Org. Biomol. Chem.* **5** (2007), 1437-1441.
136. "Dark-Red O₈ Molecules in Solid Oxygen: Rhomboid Clusters, Not S₈-Like Rings", R. Steudel and M.W. Wong, *Angew. Chem. Int. Ed.* **46** (2007) 1768-1771.
135. "Mechanism of Metal Halide-Promoted Mukaiyama Aldol Reactions", C.T. Wong and M.W. Wong, *J. Org. Chem.* **72** (2007) 1425-1430.
134. "Structures and Vibrational Spectra of the Sulfur-Rich Oxides S_nO (*n* = 4-9). The Importance of π*-π* Interaction", M.W. Wong, Y. Steudel and R. Steudel, *Chem. Eur. J.* **13** (2007) 502-514.
133. "Homolytic Dissociation of the Vulcanization Accelerator Tetramethylthiuramdisulfide (TMTD) and Structures and Stabilities of the Radicals Me₂NCS_n[•] (*n* = 1-4)", R. Steudel, Y. Steudel, A.M. Mak and M.W. Wong, *J. Org. Chem.* **71** (2006) 9302-9311.

132. "Saturated Hydrocarbon-Benzene Complexes: A Theoretical Study of Cooperative CH/ π Interaction", Ran J. and M.W. Wong, *J. Phys. Chem. A* **110** (2006) 9702-9709.
131. "S₃O₂ – An Unusual Structure with π^* - π^* Interaction", M.W. Wong, and R. Steudel, *Phys. Chem. Chem. Phys.* **8** (2006) 1292-1297.
130. "Benzyl Radical Clock kinetics Applied to Methyl Abstraction of CpFe(CO)₂Me ", T.S. Chong, T.S. Chwee, W.K. Leong, M.W. Wong and W.Y. Fan, *J. Organomet. Chem.* **691** (2006) 687-692.
129. "Preparation and Characterization of Cr(CO)₄dpp (Chromium Tetracarbonyl 2,3-bis(2'-pyridyl)Pyrazine) Adsorbed on Silver Nanoparticles ", H. Tan, L. Wong, M.Y. Lai, G.S.M. Kiruba, W.K. Leong, M.W. Wong and W.Y. Fan, *J. Phys. Chem. B* **109** (2005) 19657-19663.
128. "Isomers of *cyclo*-Heptasulfur and their Coordination to Li⁺ - An Ab Initio MO Study", M.W. Wong, Y. Steudel and R. Steudel, *Inorg. Chem.* **44** (2005) 8908-8915.
127. "Structures of the Trisulfur Oxides S₃O and S₃O⁺: Branched Rings, not Open Chains", M.W. Wong and R. Steudel, *Chem. Commun.* (2005) 3712-3714.
126. "On the Roles of C-H \cdots O=S and π -stacking Interactions in 2-Bromoacrolein Complex with *N*-tosyl-(*S*)-tryptophan Derived Oxazaborolidinone Catalyst", M.W. Wong, *J. Org. Chem.* **70** (2005) 5487-5493.
125. "Coordination of Li⁺, Ca⁺, V⁺ and Cu⁺ to the Molecules S₈ and S₄: A Computational Study", Y. Steudel, M.W. Wong and R. Steudel, *Eur. J. Inorg. Chem.* (2005) 2514-2525.
124. "Thermochemistry of Reactive Nitrogen Oxide Species and Reaction Enthalpies for Decomposition of ONOO⁻ and ONOOH", A.M. Mak and M.W. Wong, *Chem. Phys. Lett.* **403** (2005) 192-197.
123. "Electrophilic Attack on Sulfur-Sulfur Bonds: Coordination of Lithium Cations to Sulfur-Rich Molecules Studied by Ab Initio MO Method", Y. Steudel, M.W. Wong and R. Steudel, *Chem. Eur. J.* **11** (2005) 1281-1293.
122. "Facile Uncatalyzed Mukaiyama Aldol Reactions: An Ab Initio Study of the Effects of Substituents", C.T. Wong and M.W. Wong, *J. Org. Chem.* **70** (2005) 124-131.

121. "Fluoride Ion Receptors Based on Dipyrrolyl Derivatives Bearing Electron-Withdrawing Groups: Synthesis, Optical and Electrochemical Sensing and Computational studies", T. Ghosh, B.G. Maiya, and M.W. Wong, *J. Phys. Chem. A* **108** (2004) 11249-11259.
120. "Novel Isomers of Hexasulfur: Prediction of a Stable Prism Isomer and Implications for the Thermal Reactivity of Elemental Sulfur", M.W. Wong, Y. Steudel and R. Steudel, *J. Chem. Phys.* **121** (2004) 5899-5907.
119. "Electrophilic Attack on Sulfur-Sulfur Bonds I: Protonation of Various Isomers of the Homoatomic Sulfur Molecules S_n ($n = 2-8$)", M.W. Wong, T.S. Chwee and R. Steudel, *J. Phys. Chem. A* **108** (2004) 7091-7098.
118. "*Gauche/Trans* Equilibria of 2,2'-Bi-1,3-dioxepanyl and 2,2'-Bi-1,3-dithiepanyl in Different Media – Theory and Experiment", Y. Lam, M.W. Wong, G.S.M. Kiruba, H.-H. Huang and E. Liang, *J. Phys. Chem. A* **108** (2004) 6874-6878.
117. "Structure and Spectra of Tetrasulfur S_4 – An Ab Initio MO Study", M.W. Wong and R. Steudel, *Chem. Phys. Lett.* **379** (2003) 162-169.
116. "*Gauche/Trans* Equilibria of 2,2'-Bi-1,3-dioxanyl, 2,2'-Dimethyl-2,2'-bi-1,3-dioxanyl, 2,2'-Bi-1,3-dithianyl and 2,2'-Dimethyl-2,2'-bi-1,3-dithianyl in Different Media – Theory and Experiment", W. Chen, Y. Lam, M.W. Wong, H.-H. Huang and E. Liang, *J. Phys. Chem. A* **107** (2003) 6714-6719.
115. "Tautomeric Equilibria of Pyridoxal-5'-Phosphate (Vitamin B_6) and 3-Hydroxypyridine Derivatives: A Theoretical Study of Solvation Effects, G.S.M. Kiruba and M.W. Wong *J. Org. Chem.* **68** (2003) 2874-2881.
114. "*Gauche/Trans* Equilibria of 2,2'-Bi-1,3-dioxolanyl, 2,2'-Dimethyl'-bi-1,3-dioxolanyl, 2,2'-Bi-1,3-dithiolanyl and 2,2'-Dimethyl'-bi-1,3-dithiolanyl in Different Media: Theory and Experiment", W. Chen, Y. Lam, M.W. Wong, H.-H. Huang and E. Liang, *New J. Chem. A* **26** (2002) 1686-1692.
113. "2-Pyrazinylnitrene and 4-Pyrimidylnitrene. Ring Expansion to 1,3,5-Triazacyclohepta-1,2,4,6-tetraene and Ring Opening to (2-Isocyanovinyl)carbodiimide", C. Addicott, M. W. Wong and C. Wentrup, *J. Org. Chem.* **67** (2002) 8538-8546.
112. "Novel Species for the Sulfur Zoo: Isomers of S_8 ", M.W. Wong, Y. Steudel and R. Steudel, *Chem Phys. Lett.* **364** (2002) 387-392.

111. "From Molecular Complexes to Zwitterions and Final Products. Reactions Between C_3O_2 and Amines", B. Sessouma, I. Couturier-Tamburelli, M. Monnier, M.W. Wong, C. Wentrup, and J.-P. Aycard, *J. Phys. Chem. A* **106** (2002) 4489-4497.
110. "Atomic Properties of N_2O_4 Based on Its Experimental Charge Density", M. Messerschmidt, A. Wagner, M.W. Wong, and P. Luger, *J. Am. Chem. Soc.* **124** (2002) 732-773.
109. "The Thermal Decomposition of Ethylene Episuifur – A Mechanistic Study by Ab Initio MO Theory", Y. Steudel, R. Steudel and M.W. Wong, *Chem. Eur. J.* **8** (2002) 217-228.
108. "Stereochemistry of Radical Halogenation Reactions. An Ab Initio Molecular Study", Z.-H. Li, K.-N. Fan and M.W. Wong, *J. Phys. Chem. A* **105** (2001) 10890-10898.
107. "Characterization of two $C_2S_4^{++}$ Isomers by Mass Spectrometry and Ab Initio Molecular Orbital Calculations", P. Gerbaux, R. Flammang, M.W. Wong and C. Wentrup, *Int. J. Mass Spectrom.* **210** (2001) 31-42.
106. "The Thermal Fragmentation of 1,6-dioxo-6a λ -thiapentalenes: Formation of Acylthioketenes and Thioacylketenes", C. Th. Pedersen, M.W. Wong and R. Flammang, *J. Chem. Soc. Perkin Trans 2* (2001) 2047-2052.
105. "Conformational Analysis of Meso- and (\pm)-2,3-Dicyano-2,3-dicyclopropyl-butane and 1,2-Dicyanotetracyclopropylethane", Y. Lam, M.W. Wong, H.-H. Huang and E. Liang, *New J. Chem.* **25** (2001) 1325-1329.
104. "An Ab Initio MO Study of the Gas Phase Reactions $2SF_2 \rightarrow FS-SF_3 \rightarrow S=SF_4$: Molecular Structures, Reaction Enthalpies and Activations Energies", Y. Steudel, R. Steudel, M.W. Wong and D. Lentz, *Eur. J. Inorg. Chem* (2001) 2543-2548.
103. "Scaling of Correlation Basis Set Extension Energies", Z.-H. Li and M.W. Wong, *Chem. Phys. Lett.* **337** (2001) 209-216.
102. "Preparation and Chemistry of an Unexpectedly Stable α -Oxoketene-Pyridine Zwitterion 2,2-Bis(*tert*-butylcarbonyl-[4-dimethylamino]pyridino[ethen-1-olate]", G. Kollenz, S. Holzer, C.O. Kappe, T.S. Dalvi, W.M.F. Fabian, H. Sterk, M.W. Wong and C. Wentrup, *Eur. J. Org. Chem.* (2001) 1315-32.
101. "Specific Interactions in Miscible Poly(p-Vinylphenol)/Poly[(N-Methyl-3-Piperidinomethyl Methacrylate) Blends", S.H. Goh, S.Y. Lee, X. Luo, M.W. Wong, and K.L. Tan, *Macromolecular Chem. Phys.* **202** (2001) 31-35.

100. "Mesionic and Non-mesionic Pyridopyrimidinylium and Pyridooxazinylium Olates. Structures in the Solid State, Solution and Matrices", C. Plüg, B. Wallfisch, H.G. Andersen, P.v. Bernhardt, L.-J. Baker, G.R. Clark, M.W. Wong and C. Wentrup, *J. Chem. Soc. Perkin Trans 2* (2000) 2096-2108.
99. "Rotational Isomerism and Crystal Structures of 2,2'-Diphenyl-2,2-bis-dithiane and 2,2'-Diphenyl-2,2-bis-dioxolane", Y. Lam, M.W. Wong, H.-H. Huang and E. Liang, *Chem. Soc. Perkin Trans 2* (2000) 2090-2095.
98. "Prediction of a Metastable Helium Compound: HHeF", M.W. Wong, *J. Am. Chem. Soc.* **122** (2000) 6289-6290.
97. "Acylthioketene–Thioacylketene–Thiet-2-one Rearrangements", J.R. Ammann, R. Flammang, M.W. Wong and C. Wentrup, *J. Org. Chem.* **65** (2000) 2706-2710.
96. "Mono- Di- and Tri-nitrenes in the Pyridine Series", S. V. Chapyshev, A. Kuhn, M.W. Wong and C. Wentrup, *J. Am. Chem. Soc.* **122** (2000) 1572-1579.
95. "A Theoretical Study of the Properties and Reactivities of Ketene, Thioketene and Seleenketene", N.L. Ma and M.W. Wong, *Eur. J. Org. Chem.* (2000) 1411-1421.
94. "Monomer, Dimers and Trimers of Cyanogen *N*-Oxide, $N\equiv C-C\equiv N\rightarrow O$. An X-ray, FVT-MS/IR and Theoretical Investigation", M. Barbieux–Flammang, S. Vandevoorde, R. Flammang, M.W. Wong, H. Bibas, H.L. Kennard and C. Wentrup, *Chem. Soc. Perkin Trans 2* (2000) 437-438.
93. "A Stable Ketene Pyridine Pre-reactive Intermediate: Experimental and Theoretical Identifications of the $C_3O_2\cdots$ Pyridine Complex", I. Couturier-Tamburelli, J.-P. Aycard, M.W. Wong, and C. Wentrup, *J. Phys. Chem. A* **104** (2000) 3466-3471.
92. "Mesions and Ketene Valence Isomers. The Pyrrolo[1,2-*a*]pyridinium Olate and (2-Pyridyl)carbonylketenes", X. Ye, J. Andraos, H. Bibas, M.W. Wong and C. Wentrup, *J. Chem. Soc. Perkin Trans 1* (2000) 401-406.
91. "The Ring-Opening Reaction of 2-Furylcarbene: Substituent Effects", Y. Sun and M.W. Wong, *J. Org. Chem.* **64** (1999) 9170-9174.
90. "Alkoxy Isothiocyanates, $RO-N=C=S$ ", A.T. Bech, R. Flammang, C. Th. Pedersen, M.W. Wong and C. Wentrup, *J. Chem. Soc. Perkin Trans 2* (1999) 1869-1873.
89. "Formation and Characterization of Methoxy Isothiocyanate ($CH_3ON=C=S$) and Methylcyanate N-Sulfide ($CH_3OC\equiv N^+-S^-$) as Radical Cations and Neutrals in the Gas Phase", R. Flammang, P. Gerbaux, M. Barbieux–Flammang, C. Th. Pedersen,

- A.T. Bech, E.H. Mørkved, C. Wentrup, and M.W. Wong, *J. Chem. Soc. Perkin Trans 2* (1999) 1683-1688.
88. "Ab Initio Study on Thermal Decomposition of Gamma-Butyrolactone", Z.H. Li, W.N. Wang, M.W. Wong, H.H. Huang and W. Huang, *Chem. Phys. Lett.* **305** (1999) 474-482.
87. "Miscibility and Interaction in Blends and Complexes of Poly[2-dimethylamino]ethyl methacrylate] with Poly(p-vinylphenol)", X.-D. Huang, S.H. Goh, Z.D. Zhao, M.W. Wong, and C.H.A. Huan, *Macromolecules* **32** (1999) 4327-4331.
86. "Characterization of New Sulfide Ions ($C_2S_3^{*+}$) from Ethenedithione by Ion-molecule Reactions", P. Gerbaux, R. Flammang, C. Th. Pedersen and M.W. Wong, *J. Phys. Chem. A* **103** (1999) 3666-3671.
85. "Identification of Singlet and Triplet $CNOS^+$ Cations in the Gas Phase", R. Flammang, P. Gerbaux and M.W. Wong, *Chem. Phys. Lett.* **300** (1999) 183-188.
84. "Ethenedithione ($S=C=C=S$): Does it obey Hund's rule?", N.L. Ma and M.W. Wong, *Angew. Chem. Engl. Ed.* **37** (1998) 3402-3404.
83. "Nitrile *N*-Selenides ($RC\equiv NSe$) Neutrals and Radical Cations: Tandem Mass Spectrometry and Ab Initio Studies", P. Gerbaux, R. Flammang, E.H. Mørkved, M.W. Wong and C. Wentrup, *J. Phys. Chem. A* **102** (1998) 9021-9030.
82. "Thermochemistry of CH_3CN , CH_3NC and Their Cyclic Isomers, and Related Radicals, Cations and Anions: Some Curious Discrepancies Between Theory and Experiment", P. M. Mayer, M. S. Taylor, M. W. Wong and L. Radom, *J. Phys. Chem. A* **102** (1998) 7074-7080.
81. "Highly Stereoselective Indium Trichloride-Catalysed Asymmetric Aldol Reaction of Formaldehyde and a Glucose-Derived Enol Ether in Water", T.P. Loh, G.L. Chua, J.J. Vittal and M.W. Wong, *J. Chem. Soc. Chem. Commun.* (1988) 861-862.
80. "Carboxy(vinyl)ketene Intermediates in the Thermolysis of Methylthio- and Methoxy-substituted Meldrum's Acid Derivatives", H. Bibas, C.O. Kappe, M.W. Wong and C. Wentrup, *J. Chem. Soc. Perkin Trans 2* (1998) 493-498.
79. "Radical Addition to Alkenes: Further Assessment of Theoretical Procedures", M.W. Wong and L. Radom, *J. Phys. Chem. A* **102** (1998) 2237-2245.

78. "Facile 1,3-Shift of Chlorine in a Chlorocarbonylketene", J. Finnerty, J. Andraos, Y. Yamamoto, M.W. Wong and C. Wentrup, *J. Am. Chem. Soc.* **120** (1998) 1701-1704.
77. "The Prediction of Vibrational Frequencies of Inorganic Molecules Using Density Functional Theory", I. Bytheway and M.W. Wong, *Chem. Phys. Lett.* **282** (1998) 219-226.
76. "Generation of Nitrile *N*-Selenides, $RC\equiv NSe$, as Neutrals and Radical Cations in the Gas Phase", P. Gerbaux, E.H. Mørkved, R. Flammang, M.W. Wong and C. Wentrup, *Tetrahedron Lett.* **39** (1998) 533-536.
75. "Characterization of Cyanogen *N*-Oxide Radical Cation ($NCCNO^{\bullet+}$) in the Gas Phase By Tandem Mass Spectrometry Methodologies and Ab Initio Calculations", R. Flammang, M. Barbieux-Flammang, P. Gerbaux, C. Wentrup and M.W. Wong, *Bull. Soc. Chim. Belg.* **106** (1997) 545-551.
74. "Generation of New Nitrile *N*-Sulfides (RCNS) Radical Cations and Neutrals via Ion-Molecule Reactions: Tandem Mass Spectrometry and Ab Initio MO Study", P. Gerbaux, Y. Van Haverbeke, R. Flammang, M.W. Wong and C. Wentrup, *J. Phys. Chem. A* **101** (1997) 6970-6975.
73. "Cyanoketene and Iminopropadienones", D.W.J. Moloney, M.W. Wong, R. Flammang, and C. Wentrup, *J. Org. Chem.* **62** (1997) 4240-4247.
72. "Nitrilimines: Evidence for the Allenic Structure in Solution, Experimental and Ab Initio Studies of the Barrier to Racemization, and First Diastereoselective [3+2]-Cycloaddition", J.-L. Faure, R. Réau, M.W. Wong, R. Koch, C. Wentrup and G. Bertrand, *J. Am. Chem. Soc.*, **119** (1997) 2819-2824.
71. "The Vinylketene–Acylallene Rearrangement: Theory and Experiment", H. Bibas, M.W. Wong and C. Wentrup, *Chem. Eur. J.* **3** (1997) 237-248.
70. "Reactivity of Carbenes and Ketenes in Low-Temperature Matrices. Carbene CO Trapping, Wolff Rearrangement and Ketene-Pyridine Ylide (Zwitterion) Observation", P. Visser, R. Zuhse, M.W. Wong and C. Wentrup, *J. Am. Chem. Soc.* **118** (1996) 12598-12602.
69. "Synthesis of *N*-Confused Porphyrin Analogues by *b*-Azafulvenones Tetramerization", G.G. Qiao, M.W. Wong and C. Wentrup, *J. Org. Chem.* **61** (1996) 8125-8131.

68. "Generation of New Nitrile N-Sulfides (NCCNS, R₂NCNS, H₃CCNS and ClCNS) as Ions and Neutrals in the Gas Phase: Tandem Mass Spectrometry, Flash-Vacuum Pyrolysis and Ab Initio MO Study", R. Flammang, P. Gerbaux, E.H. Mørkved, M.W. Wong and C. Wentrup, *J. Phys. Chem.* **100** (1996) 17452-17459.
67. "Novel Heterocumulenes: Bisiminopropadienones and Linear Ketenimines", R. Wolf, Stefan Stadtmüller, M.W. Wong, M. Barbieux-Flammang and R. Flammang and C. Wentrup, *Chem. Eur. J.* **2** (1996) 1318-1329.
66. "Interconversions of Phenylcarbene, Cycloheptatetraene, Fullenallene and Benzocyclopropene. A Theoretical Study of C₇H₆ Energy Surface", M.W. Wong and C. Wentrup, *J. Org. Chem.* **61** (1996) 7022-7029.
65. "Facile 1,3- and 1,5-Chlorine Migration", R. Koch, M.W. Wong and C. Wentrup, *J. Org. Chem.* **61** (1996) 6809-6813.
64. "Novel Heterocumulenes (RN=C=C=C=X) and Ketene Rearrangements", C. Wentrup, B.E. Fullon, D.W.J. Moloney, H. Bibas, M.W. Wong, *Pure & Appl. Chem.* **68** (1996) 891-893.
63. "Characterization of New Cumulenes C₂NX₂ (X = O or S): Tandem Mass Spectrometry and Ab Initio Studies", M.W. Wong, C. Wentrup, E.H. Mørkved and R. Flammang, *J. Phys. Chem.* **100** (1996) 10536-10541.
62. "Cyanovinylketenes From Azafulvenones: An Apparent Retro-Wolff Rearrangement", G.G. Qiao, W. Meutermans, M.W. Wong, M. Träubel and C. Wentrup, *J. Am. Chem. Soc.* **118** (1996) 3852-3861.
61. "Vibrational Frequency Prediction Using Density Functional Theory", M.W. Wong, *Chem. Phys. Lett.* **256** (1996) 391-399.
60. "2-Pyridylnitrene-1,3-Diazacyclohepta-1,2,4,6-tetrane Rearrangements in the Trifluoro-methyl-2-pyridyl Azide Series", R.A. Evans, M.W. Wong and C. Wentrup, *J. Am. Chem. Soc.* **118** (1996) 4009-4017.
59. "An Unexpected Effect of the Nature of the Collision Gas in Collisional Activation Mass Spectrometry", R. Flammang, L. Gallez, Y. Van Haverbeke, M.W. Wong and C. Wentrup, *Rapid Commun., Mass Spectrom.* **10** (1996) 232-234.
58. "Photochemistry of Deuterated Acetylketene: Matrix Isolation Infrared Spectroscopic and Ab Initio Studies", R. Zuhse, M.W. Wong and C. Wentrup, *J. Phys. Chem.* **100** (1996) 3917-3922.

57. "Polycarbon Disulfides SC_nS ($n = 1-3$) and their Protonated and Methylated Forms ($HC_nS_2^+$ and $CH_3C_nS_2^+$): Tandem Mass Spectrometry and Ab Initio MO Study", M.W. Wong, R. Flammang and C. Wentrup, *J. Phys. Chem.* **99** (1995) 16849-16856.
56. "Structures and Stabilities of Gas-Phase $C_6H_4X^-$ ($X = F, Cl$ and Br) Anions: Benzyne-Halide Ion Complexes?", M.W. Wong, *J. Chem. Soc. Chem. Commun.* (1995) 2227-2228.
55. "Vinylketene-Acylallene Rearrangement", H. Bibas, M.W. Wong and C. Wentrup, *J. Am. Chem. Soc.* **117** (1995) 9582-9583.
54. "Structures and Stabilities of $XCCY^{2+}$ Dications ($X, Y = O, S$ and NH), Doubly Charged Isoelectronic Analogues of Cyanogen", M.W. Wong, *J. Mass Spectrom.* **30** (1995) 1144-1148.
53. "A Remarkably Stable Ketenimine", R. Wolf, M.W. Wong, C. H. L. Kennard and C. Wentrup, *J. Am. Chem. Soc.* **117** (1995) 6789-6790.
52. "Radical Addition to Alkenes: An Assessment of Theoretical Procedures", M.W. Wong, and L. Radom, *J. Phys. Chem.* **99** (1995) 8582-8588.
51. "Polycarbon Sulfides C_nS ($n=2-6$) and Corresponding Hydrides HC_nS^\bullet . Neutralization-Reionization Mass Spectrometry and Ab Initio Molecular Orbital Study", R. Flammang, Y. van Haverbeke, M.W. Wong and C. Wentrup, *Rapid Commun., Mass Spectrom.* **9** (1995) 203-208.
50. "The Use of 1,2-shifts in Carbenes and Nitrenes in the Generation of Novel Heterocumulenes", C. Wentrup, C.O. Kappe and M.W. Wong, *Pure & Appl. Chem.* **67** (1995) 749-754.
49. "Acetylketene: Conformational Isomerism and Photochemistry. Matrix Isolation Infrared and Ab Initio Studies", C.O. Kappe, M.W. Wong and C. Wentrup, *J. Org. Chem.* **60** (1995) 1686-1695.
48. "Ab Initio Calculation of Molar Volumes: Comparison with Experiment and Use in Solvation Models", M.W. Wong, K.B. Wiberg and M.J. Frisch, *J. Comput. Chem.* **16** (1995) 385-394.
47. "Addition of *tert*-Butyl Radical to Substituted Alkenes: A Theoretical Study of the Reaction Mechanism", M.W. Wong, A. Pross and L. Radom, *J. Am. Chem. Soc.*, **116** (1994) 11938-11943.

46. "Ketene-Ketene Rearrangement: Substituent Effects on the 1,3-Migration in α -Oxoketenes", M.W. Wong and C. Wentrup, *J. Org. Chem.*, **59** (1994) 5279-5285.
45. "Iminoethenone Radical Cations ($\text{RN}=\text{C}=\text{C}=\text{O}^{\bullet+}$) : Tandem Mass Spectrometry and Ab Initio MO Studies", R. Flammang, Y. van Haverbeke, S. Laurent, M. Barbieux-Flammang, M.W. Wong and C. Wentrup, *J. Phys. Chem.* **98** (1994) 5801-5806.
44. "Protonated Forms of Iminopropadienones, $\text{RN}=\text{C}=\text{C}=\text{C}=\text{O}$, and Cyanoketenes: Combined Ab Initio MO and Mass Spectrometry Studies", R. Flammang, Y. van Haverbeke, M.W. Wong, A. Rühmann and C. Wentrup, *J. Phys. Chem.* **98** (1994) 4814-4820.
43. "Comparison of the Addition of CH_3^{\bullet} , $\text{CH}_2\text{OH}^{\bullet}$ and $\text{CH}_2\text{CN}^{\bullet}$ Radicals to Substituted Alkenes: A Theoretical Study of the Reaction Mechanism", M.W. Wong, A. Pross and L. Radom, *J. Am. Chem. Soc.* **116** (1994) 6284-6292.
42. "Iminoethenethiones, $\text{RN}=\text{C}=\text{C}=\text{S}$: Characterization by Neutralization-Reionization Mass Spectrometry and G2(MP2) Theory", R. Flammang, D. Landu, S. Laurent, M. Barbieux-Flammang, C.O. Kappe, M.W. Wong and C. Wentrup, *J. Am. Chem. Soc.* **116** (1994) 2005-2013.
41. "Iminopropadienones, $\text{RN}=\text{C}=\text{C}=\text{C}=\text{O}$: Theory and Experiment", T. Mosandl, S. Stadtmüller, M.W. Wong and C. Wentrup, *J. Phys. Chem.* **98** (1994) 1080-1086.
40. "Matrix Isolation and Infrared Spectrum of Thioformyl Cyanide", C.O. Kappe, M.W. Wong and C. Wentrup, *Tetrahedron Lett.* (1993) 6623-6626.
39. "Structure of Nitrilimine: Allenic or Propargylic?", M.W. Wong and C. Wentrup, *J. Am. Chem. Soc.* **115** (1993) 7743-7746.
38. "Tautomeric Equilibrium and Hydrogen Shifts of Tetrazole in the Gas Phase and in Solution", M.W. Wong, R. Leung-Toung and C. Wentrup, *J. Am. Chem. Soc.* **115** (1993) 2465-2472.
37. "Addition of Methyl Radical to Substituted Alkenes: A Theoretical Study of the Reaction Mechanism", M.W. Wong, A. Pross and L. Radom, *Isr. J. Chem. Soc.* **33** (1993) 415-425.
36. "Scaling Factors for Obtaining Fundamental Vibrational Frequencies and Zero-Point Energies from HF/6-31G* and MP2/6-31G* Harmonic Frequencies", J.A. Pople, A.P. Scott, M.W. Wong and L. Radom, *Isr. J. Chem. Soc.* **33** (1993) 345-350.

35. "Are Polar Interactions Important in the Addition of Methyl Radical to Alkenes", M.W. Wong, A. Pross and L. Radom, *J. Am. Chem. Soc.* **115** (1993) 11050-11051.
34. "Thermochemistry and Ion-Molecule Reactions of Isomeric C₃H₂^{•+} Cations", M.W. Wong and L. Radom, *J. Am. Chem. Soc.* **115** (1993) 1507-1514.
33. "Theoretical Investigation of the Rotational Barrier in Allyl and 1,1,3,3-Tetramethylallyl Ions", J.B. Foresman, M.W. Wong, K.B. Wiberg and M.J. Frisch, *J. Am. Chem. Soc.* **115** (1993) 2220-2226.
32. "Solvents Effects. 4. Effect of Solvent on the *E/Z* Energy Difference for Methyl Formate and Methyl Acetate", K.B. Wiberg and M.W. Wong, *J. Am. Chem. Soc.* **115** (1993) 1078-1084.
31. "Helides of Carbon and Silicon: An Ab Initio Study of Their Geometric and Electronic Structures", E.D. Jemmis, M.W. Wong, H.-B. Burgi and L. Radom, *J. Mol. Struct. (Theochem)* **261** (1992) 385-401.
30. "Structures, Bonding, Absorption Spectra of Amine-Sulfur Dioxide Charge-Transfer Complexes", M.W. Wong and K.B. Wiberg, *J. Am. Chem. Soc.*, **114** (1992) 7527-7535.
29. "Structure of Acetamide: Planar or Nonplanar?", M.W. Wong and K.B. Wiberg, *J. Phys. Chem.* **96** (1992) 668-671.
28. "Solvents Effects. 3. Tautomeric Equilibria of Formamide and 2-Pyridone in the Gas Phase and Solution. An Ab Initio SCRF Study", M.W. Wong, K.B. Wiberg and M.J. Frisch, *J. Am. Chem. Soc.* **114** (1992) 1645-1652.
27. "Solvent Effects. 2. Medium Effect on the Structure, Energy, Charge Density, and Vibrational Frequencies of Sulfamic Acid", M.W. Wong, K.B. Wiberg and M.J. Frisch, *J. Am. Chem. Soc.* **114** (1992) 523-529.
26. "Hartree-Fock Second Derivatives and Electric Field Properties in a Solvent Reaction Field: Theory and Application", M.W. Wong, K.B. Wiberg and M.J. Frisch, *J. Chem. Phys.* **95** (1991) 8991-8998.
25. "Solvent Effects. 1. The Mediation of Electrostatic Effects by Solvents", M.W. Wong, M.J. Frisch and K.B. Wiberg, *J. Am. Chem. Soc.* **113** (1991) 4776-4782.
24. "The Structure and Stability of the O₂²⁺ Dication: A Dramatic Failure of Møller-Plesset Perturbation Theory", R.H. Nobes, D. Moncrieff, M.W. Wong, L. Radom, P.M.W. Gill and J. Pople, *Chem. Phys. Lett.* **182** (1991) 216-224.

23. "Two-Electron Integral Evaluation for Uncontracted Geometrical-Type Gaussian Functions", M.W. Wong, G. Corongiu and E. Clementi, *J. Comput. Chem.*, **12** (1991) 215-219.
22. "Isoelectronic Analogues of PN: Remarkably Stable Multiply Charged Cations", M.W. Wong and L. Radom, *J. Phys. Chem.*, **94** (1990) 638-644.
21. "A Theoretical study of the C₃H₄²⁺ Potential Energy Surface", M.W. Wong and L. Radom, *J. Mol. Struct.* **198** (1989) 391-401.
20. "Multiply-Charged Isoelectronic Analogues of C₃H₃⁺: Cyclic or Open-Chain?", M.W. Wong and L. Radom, *J. Am. Chem. Soc.* **111** (1989) 6976-6983.
19. "Structures and Stabilities of [C₃H₂]^{•+} and [C₃H₂]²⁺ Ions", M.W. Wong and L. Radom, *Org. Mass Spectrom.* **24** (1989) 539-545.
18. "Neutralization-Reionization of CH₄^{•+}: At Which Stage Does Fragmentation Occur?", C.E.C.A. Hop, J.L. Holmes, M.W. Wong and L. Radom, *Chem. Phys. Lett.* **159** (1989) 580-586.
17. "Multiply-Bonded Argon-Containing Ions: Structures and Stabilities of XArⁿ⁺ Cations (X=B, C and N; n = 1-3)", M.W. Wong and L. Radom, *J. Phys. Chem.* **93** (1989) 6303-6308.
16. "Isoelectronic Analogs of Molecular Nitrogen: Tightly-Bound Multiply-Charged Species", M.W. Wong, R.H. Nobes, W.J. Bouma and L. Radom, *J. Chem. Phys.* **91** (1989) 2971-2979.
15. "Structure and Stability of the Tetrahydroselenonium Dication SeH₄²⁺", M.W. Wong and L. Radom, *Struct. Chem.* **1** (1989) 13-18.
14. "The HCNArF⁺ Cation: Prediction of a Stable Argon-Nitrogen Bonded Species", M.W. Wong and L. Radom, *J. Chem. Soc., Chem. Commun.* (1989) 719-721.
13. "Methane Dication: Planar but not Square", M.W. Wong and L. Radom, *J. Am. Chem. Soc.* **111** (1989) 1155-1156.
12. "The Vinyl Dication (CH₂CH^{•2+}): Classical or Bridged?", M.W. Wong and L. Radom, *Int. J. Mass Spectrom. Ion Proc.* **86** (1988) 319-327.
11. "How Well can RMP4 Theory Treat Homolytic Fragmentations?", P.M.W. Gill, M.W. Wong, R.H. Nobes and L. Radom, *Chem. Phys. Lett.* **148** (1988) 541-549.

10. "6-311G(MC)(d,p): A Second Row Analogue of the 6-311G(d,p) Basis Set. Calculated Heats of Formation of Second-Row Hydrides", M.W. Wong, P.M.W. Gill, R.H. Nobes and L. Radom, *J. Phys. Chem.* **92** (1988) 4875-4880.
9. "Remarkable Stabilities of the Diatomic Multiply-Charged Cations SiHe³⁺ and SiHe⁴⁺", M.W. Wong and L. Radom, *J. Am. Chem. Soc.* **110** (1988) 2375-2378.
8. "Multiply-Charged Cations: Remarkable Structures and Stabilities", L. Radom, P.M.W. Gill, M.W. Wong and R.H. Nobes, *Pure Appl. Chem.* **60** (1988) 183-188.
7. "The [HCS]⁺ and [H₂CS]²⁺ Potential Energy Surfaces: Predictions of Bridged Equilibrium Structures", M.W. Wong, R.H. Nobes and L. Radom, *J. Mol. Struct. (Theochem)* **163** (1988) 151-161.
6. "The Structure of the C₂H₄²⁺ Dication", R.H. Nobes, M.W. Wong and L. Radom, *Chem. Phys. Lett.* **136** (1987) 299-302.
5. "Multiply-Charged Helium-Containing Cations: HeCO²⁺, HeCF³⁺ and HeCNe⁴⁺", M.W. Wong, R.H. Nobes and L. Radom, *Rapid Commun., Mass Spectrom.* **1** (1987) 3-5.
4. "Substituted Methylene Dications (HCX²⁺): Some Remarkably Short Bonds to Carbon", M.W. Wong, B.F. Yates, R.H. Nobes and L. Radom, *J. Am. Chem. Soc.* **109** (1987) 3181-3187.
3. "The Ethyl Dication (CH₃CH₂²⁺): Classical (Open) or Non-Classical (Bridged)?", M.W. Wong, J. Baker, R.H. Nobes and L. Radom, *J. Am. Chem. Soc.* **109** (1987) 2245-2250.
2. "Remarkably Stable Trications and Tetracations: The Triheliomethyl Trication (CHe₃³⁺) and Tetraheliomethane Tetracation (CHe₄⁴⁺)", M.W. Wong, R.H. Nobes and L. Radom, *J. Chem. Soc., Chem. Commun.* (1987) 233-234.
1. "Pyrolysis of Aryl Azides VI. Identification of Neighbouring Group Effects in Pyrolysis of Azidopyridines and Azidoquinolines", L.K. Dyllal and M.W. Wong, *Aust. J. Chem.* **38** (1985) 1045-1059.

Chapters in Books

7. "Quantum-Chemical Calculations of Sulfur-Rich Compounds", M.W. Wong, *Top. Curr. Chem.* **231** (2003) 1-30.

6. "Speciation and Thermodynamics of Sulfur Vapor", R. Steudel, Y. Steudel and M.W. Wong, *Top. Curr. Chem.* **230** (2003) 117-134.
5. "Radical Addition to Alkenes: A Theoretical Perspective", L. Radom, M.W. Wong, and A. Pross, in *Controlled Radical Polymerization. ACS Symposium Series 685*, K. Matyjaszewski, Ed., American Chemical Society, 1998, Washington DC, p.31-49.
4. Ketene Rearrangements and 1,3-Shifts", C. Wentrup and M.W. Wong, in *Atualidades de Fisico-Quimica Organica*, J. J. E. Humeres, Ed., Florianopolis, Santa Catarina, Brasil, 1995, p.48-62.
3. "Structural and Energetic Consequences of Single and Double Ionization", L. Radom, M.W. Wong and P.M.W. Gill, in *Advances in Mass Spectrometry, Volume 11A*, New York, Wiley, 1989, p.702-712.
2. "Fragmentation Mechanisms for Multiply-Charged Cations", L. Radom, P.M.W. Gill and M.W. Wong, in *The Structure of Small Molecules and Ions*, R. Naaman and Z. Vager Eds., Plenum, New York, 1989, p.219-225.
1. "Simple Models for Describing the Fragmentation Behavior of Multiply-Charged Cations", L. Radom, P.M.W. Gill and M.W. Wong, in *International Journal of Chemistry: Quantum Chemistry Symposium Volume 22*, New York, John Wiley & Sons, 1988) pp.567-573.