

David R. Yarkony
Publications: Complete

Festschrift

1. David R. Yarkony, *J. Phys. Chem. A* 118(51) 11837 (2014)

Perspective

1. *Accurate Nonadiabatic Dynamics*
Hua Guo and David R. Yarkony, *Phys. Chem. Chem Phys.* 18, 26335-26352 (2016)

Edited Books

4. *Conical Intersections, Theory Computation, Experiment*, eds. Wolfgang Domcke, David R. Yarkony and Horst Köppel, World Scientific Publishing, (Singapore, 2011),
3. *The Jahn-Teller Effect. Fundamentals and Implications for Physics and Chemistry*
editors, Horst Köppel, Heinz Barentzen, David R. Yarkony (Springer, 2009)
2. *Conical Intersections: Electronic Structure, Dynamics and Spectroscopy*, eds. Wolfgang Domcke, David R. Yarkony and Horst Köppel, World Scientific Publishing, (Singapore, 2004),
1. *Modern Electronic Structure Theory*, ed. D. R. Yarkony (World Scientific, Singapore, 1995)(Parts 1 and 2)

Journal Articles/Book Chapters

223. *Nonadiabatic tunneling via conical intersections and the role of the geometric phase*
Xie, C.; Yarkony, D. R.; Guo, H. *Phys. Rev. A* 95, 022104 (2017)
222. *On the Incorporation of the Geometric Phase in General Single Potential Energy Surface Dynamics: A Removable Approximation to Ab Initio Data*
Christopher L. Malbon, Xiaolei Zhu, Hua Guo and David R. Yarkony, *J. Chem. Phys.* 145, 234111 (2016)
221. *An Improved Quasi-Diabatic Representation of the 1,2,3 IA Coupled Adiabatic Potential Energy Surfaces of Phenol in the Full 33 Internal Coordinates.*
Xiaolei Zhu, Christopher L. Malbon and David R. Yarkony, *J. Chem. Phys.* 144, 124312 (2016)
220. *Constructing Diabatic Representations Using Adiabatic and Approximate Diabatic Data. Coping with Diabolical Singularities*
Zhu, X.; Yarkony, D. R. *J. Chem. Phys.* **144**, (2016).
219. *On the Elimination of the Electronic Structure Bottleneck in On the Fly Nonadiabatic Dynamics for Small to Moderate Sized (10-15 atom) Molecules Using Fit Diabatic Representations Based Solely on ab initio Electronic Structure Data: The Photodissociation of Phenol*
Zhu, X.; Yarkony, D. R. *J. Chem. Phys.* 144, 024105 (2016)
218. *On the Construction of Property Based Diabatizations. Diabolical Singular Points*
Zhu, X.; Yarkony, D. R. *J. Phys. Chem. A* **2015**, 119, 12383.

217. *On the Nonadiabatic Photodissociation of the Hydroxymethyl Radical from the 2^2A State. Surface Hopping Simulations Based on a Full Nine Dimensional Representation of the $1,2,3^2A$ Potential Energy Surfaces Coupled by Conical Intersections*
Christopher L. Malbon and David R. Yarkony, J. Phys. Chem. A 119, 7498-7509 (2015)
216. *Communication: On the competition between adiabatic and nonadiabatic dynamics in vibrationally mediated ammonia photodissociation in its A band.*
Xie, C.; Zhu, X.; Ma, J.; Yarkony, D. R.; Xie, D.; Guo, H.; J. Chem. Phys **2015**, 142, 091101.
215. *On the Electronic Structure of the Ground State of Cyclopentoxy. The Case for a Two Coupled State Description*
Christopher L. Malbon, David R. Yarkony, and Xiaolei Zhu, J. Mol. Spec, 311, 36-41 (2015)

214. *On the Description of Conical Intersections: A Continuous Representation of the Local Topography of Seams of Conical Intersection of Three or More Electronic States. A Generalization of the Two State Result*
Xiaolei Zhu and David R. Yarkony, *J. Chem. Phys.* **141**,174109 (2014)
213. *Full-dimensional Quantum Dynamics of Vibrationally Mediated Photodissociation of NH₃ and ND₃ on Coupled Ab Initio Potential Energy Surfaces: Absorption Spectra and NH₂(²A₁)/NH₂(X²B₁) Branching Ratios* Jianyi Ma, Changjian Xie, Xiaolei Zhu, David R. Yarkony, Daiqian Xie and Hua Guo, *J. Phys. Chem. A* (2014) (this special issue)
212. *Full-dimensional quantum state-to-state non-adiabatic dynamics for photodissociation of ammonia in its A-band* Changjian Xie, Jianyi Ma, Xiaolei Zhu, Dong Hui Zhang, David R. Yarkony Daiqian Xie and Hua Guo, *J. Phys. Chem. Lett.* **5**, 1055-1060 (2014)
211. *Fitting Coupled Potential Energy Surfaces for Large Systems: Method and Construction of a 3-State Representation for Phenol Photodissociation in Full 33 Degrees of Freedom using Multireference Configuration Interaction Determined Data*
Xiaolei Zhu, and D. R. Yarkony, *J. Chem. Phys.* **140**, 024112 (2014)
210. *On the Photoionization Spectrum of Propyne. A fully ab initio Simulation of the Low-Energy Spectrum including the Jahn-Teller Effect and the Spin-Orbit Interaction*
Sara Marquez, Joseph Dillon and David R. Yarkony, *J. Phys. Chem A.* **117**, 12002-12010 (2013)
209. *On the Electronic Structure of the Low Lying Electronic States of Vanadium Trioxide*, Elizabeth M. Y. Lee, Xiaolei Zhu and David R. Yarkony, *J. Chem. Phys.* **139**, 044303 (2013)
208. *On the Mechanism for the Nonadiabatic Reactive Quenching of OH(A²Σ⁺) by H₂(¹Σ⁺_g). The Role of the 2²A State*
Joseph Dillon and David R. Yarkony, *J. Chem. Phys.* **139**, 064314 (2013).
207. *Seams of Conical Intersections Relevant to the Quenching of OH(A²Σ⁺) by Collisions with H₂.*
Joseph Dillon and David R. Yarkony, *J. Phys. Chem. A*, **117** , 7344-7355 (2013)
206. *Nonadiabatic Quantum Chemistry- Past, Present and Future* David R. Yarkony, *Chemical Reviews*, **112** 481-498, 2012. <http://pubs.acs.org/doi/full/10.1021/cr2001299>
205. *Role of Conical Intersections in Molecular Spectroscopy and Photoinduced Chemical Dynamics*
Wolfgang Domcke, and David R. Yarkony, *Annual Reviews of Physical Chemistry*, **63**: 325 (2012).

204. *Reactive quenching of OH A $^2\Sigma^+$ by O₂ and CO: Experimental and nonadiabatic theoretical studies of H- and O-atom product channels*
Julia H. Lehman, Marsha I. Lester, and David R. Yarkony, J. Chem. Phys. **137**, 094312 (2012)
203. *First principles determination of the NH₂/ND₂(A, \tilde{X}) branching ratios for photodissociation of NH₃/ND₃ via full-dimensional quantum dynamics based on a new quasi-diabatic representation of coupled ab initio potential energy surfaces*
Jianyi Ma, Xiaolei Zhu, Hua Guo and David R. Yarkony. J. Chem. Phys. **137**, 22A541 (2012)
202. *Quasi-Diabatic Representations of Adiabatic Potential Energy Surfaces Coupled by Conical Intersections including Bond Breaking. A More General Construction Procedure and an Analysis of the Diabatic Representation*
Xiaolei Zhu and David R. Yarkony, J. Chem. Phys. **137**, 22A511 (2012)
201. *Nonadiabatic Effects in Substitutional Isomers of Jahn-Teller Molecules. The Strange Case of Hydroxymethoxy*
Joseph Dillon and David R. Yarkony, J. Chem. Phys. **137**, 154315 (2012)
200. *Computational Determination of the \tilde{A} State Absorption Spectrum of NH₃ and of ND₃ using a New Quasi Diabatic Representation of the \tilde{X} and \tilde{A} States and Full Six Dimensional Quantum Dynamics*
Xiaolei Zhu, JianYi Ma, David R. Yarkony and Hua Guo J. Chem. Phys. **136**, 234301 (2012). □
199. *A Lippmann – Schwinger Approach for the Determination of Photoionization and Photodetachment Cross Sections Based on a Partial Wave Green’s Function Expansion and Configuration Interaction Wave Functions.*
Seungsuk Han and David R. Yarkony, Mol. Phys. **110**, 845-859 (2012). □ □
198. *Determining Partial Differential Cross Sections for Low-Energy Electron Photodetachment involving Conical Intersections using the Solution of a Lippmann-Schwinger Equation Constructed with Standard Electronic Structure Techniques*
Seungsuk Han and David R. Yarkony, J. Chem. Phys. **134**, 174104 (2011)
197. *On the Simulation of Photoelectron Spectra Complicated by Conical Intersections: Higher-Order Effects and Hot Bands in the Photoelectron Spectrum of Triazolide (CH)₂N₃⁻*
Joseph Dillon, David R. Yarkony and Michael S. Schuurman, J. Chem. Phys. **134**, 184314(13 pages) (2011)
196. *On the Representation of Coupled Adiabatic Potential Energy Surfaces using Quasi-Diabatic Hamiltonians: Improved Accuracy from Geometrically Distributed Expansions*
Xiaolei Zhu and David R. Yarkony, J. Chem. Phys. **136**, 174110 (2012)

195. *Conical intersections in electron photodetachment spectroscopy: Theory and Applications*
Michael S. Schuurman and David R. Yarkony, in *Conical Intersections Theory, Application, Experiment*, Wolfgang Domcke, David R. Yarkony and Horst Köppel, eds. World Scientific Publishing, Singapore, (2011)
194. *On the Construction of Quasi Diabatic State Representations of Bound Adiabatic State Potential Energy Surfaces Coupled by Conical Intersections. Incorporation of Higher Order Terms*
Joseph J. Dillon, David R. Yarkony and Michael S. Schuurman, J. Chem. Phys. **134**, 044101 (2011).
193. *Partial Differential Photodetachment and Photoionization Cross Sections for Polyatomic Molecules with Electronic States Coupled by Conical Intersections*
S. Han and D. R. Yarkony, J. Chem. Phys., **134**, 134110 (2011)
192. *On the Role of Conical Intersections and their Local Topography in the Photodissociation of I-Hydroxyethyl Radical*,
Kousik Samanta and David R. Yarkony, Chem. Phys. **378**, 110-117 (2010)
191. *On the Representation of Coupled Adiabatic Potential Energy Surfaces using Quasi-Diabatic Hamiltonians: Description of Accidental Seams of Conical Intersection*
Xiaolei Zhu and David R. Yarkony, Molec. Phys. 108, 2611-2619 (2010)
190. *On the Determination of Intensities for Electron Photodetachment and Photoionization Spectra Involving States Coupled by Conical Intersections: Total Cross Sections for Polyatomic Molecules.*
Seungsook Han and David R. Yarkony, J. Chem. Phys., **133**, 194107 (2010)
189. *Toward the Elimination of the Electronic Structure Bottleneck in Nonadiabatic Dynamics on the Fly. A Method to Construct Nonlocal, Quasi-Diabatic, Coupled Electronic State Hamiltonians from ab initio Electronic Structure Data.*
Xiaolei Zhu and David R. Yarkony, J. Chem. Phys. **132**, 104101 (2010)
188. *The Photoelectron Spectrum of the Ethoxide Anion: Conical Intersections, the Spin-Orbit Interaction and Sequence Bands*
Joseph J. Dillon and David R. Yarkony, J. Chem. Phys. **131**, 134303 (12-pages) (2009)
187. *The simulated spectrum of isopropoxide. Nonadiabatic effects due to conical intersections and the spin-orbit interaction*
Joseph J. Dillon and David R. Yarkony, J. Chem. Phys. 130, 154312 (11 pages) (2009)
186. *The Photoelectron Spectrum of Pyrrolide: Nonadiabatic effects due to Conical Intersections*
Xiaolei Zhu and David R. Yarkony, J. Phys. Chem. C 114, 5312-5320 (2010) published on line 20 October, 2009
185. *On the Determination of Optimized, Fully Quadratic, Coupled State Quasi Diabatic*

Hamiltonians for Determining Bound State Vibronic Spectra

Xiaolei Zhu and David R. Yarkony, J. Chem. Phys. 130, 234108 (11 pages) (2009)

184. *The Simulated Photoelectron Spectrum of 1-propynide.*
Brian N. Papas, Michael S. Schuurman and David R. Yarkony, J. Chem. Phys. **130**, 064306 (12 pages) (2009).
183. *Determining quasi diabatic coupled electronic state Hamiltonians using derivative couplings. A normal equations based method.*
Brian N. Papas, Michael S. Schuurman, and David R. Yarkony, J. Chem. Phys. **129**, 24104 (10 pages) (2008)
182. *A simulation of the photoelectron spectrum of pyrazolide,*
Michael S. Schuurman and David R. Yarkony, J. Chem. Phys, **129** 064304 (14pages) (2008).
181. *A method to reduce the size of the vibronic basis employed in the simulation of spectra using the multimode vibronic coupling approximation*
Michael S. Schuurman and David R. Yarkony, J. Chem. Phys. **128** 044119 (9 pages) (2008)
180. *On the Multimode Quadratic Vibronic Coupling Model. An Open-ended Solution to the Secular Problem Using a Parallel Lanczos Algorithm*
Michael S. Schuurman, Richard A. Young and David R. Yarkony, Chem. Phys. **347**, 57-64 (2008)
179. *On the Vibronic Coupling Approximation: A Generally Applicable Approach for Determining Fully Quadratic Quasi Diabatic Coupled Electronic State Hamiltonians*
Michael S. Schuurman and David R. Yarkony, J. Chem. Phys. **127** 094104 (9 pages) (2007).
178. *On the simulation of photoelectron spectra in molecules with conical intersections and spin-orbit coupling: The vibronic spectrum of CH₃S.*
Michael S. Schuurman, Daniel E. Weinberg and David R. Yarkony, J. Chem. Phys, **127**, 104309,(12 pages) (2007)
- 177 *Interpolation of diabatic potential-energy surfaces: Quantum dynamics on ab initio surfaces*
C. R. Evenhuis, X. Lin, D. H. Zhang, D. Yarkony, and M. A. Collins, J. Chem. Phys. **123**, 134110 (2005).
176. *Seam near Seams: The Jahn-Teller Effect in the ¹E'' State of N₃⁺*
Joseph J. Dillon and David R. Yarkony, J. Chem. Phys. **126** 124113(7 pages) (2007)
175. *On the Locus of Points of Conical Intersection: Seams Near Seams*
Michael S. Schuurman and David R. Yarkony, J. Chem. Phys. 126, 044104 (2007)

174. *Towards a Highly Efficient Theoretical Treatment of Jahn-Teller Effects in Molecular Spectra: The 1^2A , 2^2A Electronic States of the Ethoxy Radical*
R. Andrew Young, Jr. and David R. Yarkony, J. Chem. Phys. 125, 234301 (2006)
173. *On the Characterization of Three State Conical Intersections using a Group Homomorphism Approach: Mapping the Full N- 5 Dimensional Seam Space*
Michael S. Schuurman and David R. Yarkony, J. Chem. Phys. 124, 244103 (2006)
172. *On the Characterization of Three State Conical Intersections Using a Group Homomorphism Approach: The Two State Degeneracy Spaces*
Michael S. Schuurman and David R. Yarkony, J. Phys. Chem. 101, 19031 (2006)
171. *On the Characterization of three state conical intersection: A Quasi Analytical Theory Using a Group Homomorphism Approach*
Michael S. Schuurman and David R. Yarkony, J. Chem. Phys. **124**, 124109(2006)
170. *A Continuous Representation of 2, 3 and 5 Dimensional Branching Spaces of Two State Conical Intersections Along their Seams*
Seung Suk Han and David R. Yarkony, in Conical Intersections, G. Worth and S. Althorpe, eds. (CCP6, London, 2005)
169. *On the Connectivity of Seams of Conical Intersection. Seam Curvature*
David R. Yarkony, J. Chem. Phys., **123** 204101(2005).
168. *A Novel Conical Intersection Topography and its Consequences. The $1, 2^2A$ Conical Intersection Seam of the Vinyloxy Radical,*
R. Andrew Young, Jr. and David R. Yarkony, J. Chem. Phys. **123**, 084315(2005)..
167. *Escape from the Double Cone: Optimized Descriptions of the Seam Space Using Gateway Modes*
David R. Yarkony, J. Chem. Phys. **123**, 134106 (2005).
166. *Statistical and Nonstatistical Nonadiabatic Photodissociation from the first excited state of the hydroxymethyl radical*
David R. Yarkony, J. Chem. Phys. **112**, 084316 (2005)
165. *Determination of potential energy surface intersections and derivative couplings in the adiabatic representation* David. R. Yarkony, in Conical Intersections: Electronic Structure, Dynamics and Spectroscopy, Wolfgang Domcke, David R. Yarkony and Horst Köppel, eds. World Scientific Publishing, Singapore, (2004)
164. *Conical Intersections: Their description and consequences*, David. R. Yarkony, in Conical Intersections: Electronic Structure, Dynamics and Spectroscopy, Wolfgang Domcke, David R. Yarkony and Horst Köppel, eds. World Scientific Publishing, Singapore, (2004).
- *163. Exploring Molecular Complexity: The Role of Conical Intersections in NH_3 Photodissociation

- David R. Yarkony, *J. Chem. Phys.* **121**,628-631(2004)
162. *Quantitative Detection of Singlet O₂ via Cavity Enhanced Absorption*
Skip Williams, Manish Gupta, Thomas Owano, Douglas S. Baer, ,Anthon y O'Keefe,
David R. Yarkony, and Spiridoula Matsika, *Optics Lett.* **29**,1066-1068(2004)
161. *Marching along ridges. Efficient location of energy minimized conical intersections of two states using extrapolatable functions*
D. R. Yarkony, *J. Phys. Chem. A* **108**, 3200-3205 (2004).
160. *Marching along ridges. An extrapolatable approach to locating conical intersections*
D. R. Yarkony, *Faraday Discussions* **127**, 325 (2004).
159. *The analytic evaluation of nonadiabatic coupling terms at the MR-CI level I; Determination of minima on the crossing seam*
Dallos, M.; Lischka, H.; Szalay, P.; Shepard, R.; Yarkony, D. R. *J. Chem. Phys.* **120** 7330(2004).
158. *The analytic evaluation of nonadiabatic coupling terms at the MR-CI level I: Formalism*
Lischka, H.; Dallos, M.; Szalay, P.; Yarkony, D. R.; Shepard, R. *J. Chem. Phys.* **120**,7322-7329 (2004).
- 157.* *Conical Intersections of Three Electronic States Affect the Ground State of Radical Species with little or no Symmetry. I. Pyrazolyl*
S. Matsika and D. R. Yarkony, *J. Amer. Chem. Soc.* **125** 12428-12429 (2003)
156. *On the properties of conical intersections of three states. Energies and the geometric phase effect in degenerate subspaces. Application to the allyl radical.*
Seungsook Han and David R. Yarkony, *J. Chem. Phys.* **119**, 5058 (2003)
155. *Beyond two-state conical intersections. Three-state conical intersections in low symmetry molecules: The allyl radical*
S. Matsika and D. R. Yarkony, *J. Amer. Chem. Soc.* **125**, 10672-10676 (2003)
154. *Nonadiabatic Processes involving Three Electronic States: I. Branch Cuts and Linked Pairs of Conical Intersections,*
Seungsook Han and David R. Yarkony, *J. Chem. Phys.* **119**, 5058-5068 (2003)
153. *On the Properties of the Seam and Branching Spaces of Conical Intersections in Molecules with an odd number of electrons: A Group Homomorphism Approach.*
Seungsook Han and David R. Yarkony, *J. Chem. Phys.* **118**, 9952 - 9962(2003)
152. *Conical Intersections and the Spin-Orbit Interaction,* Spiridoula Matsika and David R. Yarkony, in *The Role of Degenerate States in Chemistry, Advances in Chemical Physics*, Michael Baer and Gert. D. Billing, eds, J. Wiley, New York, 2002, pp. 557-583
- 151.* *Accidental Conical Intersections of three states of the same symmetry: Location and Relevance*

- S. Matsika and D. R. Yarkony, *J. Chem. Phys.* **117**, 6907-6910 (2002)
150. *Photodissociation of the vinyloxy radical through conical and avoided intersections*
S. Matsika and D. R. Yarkony, *J. Chem. Phys.* **117**, 7198 (2002)
149. *Spin-orbit Coupling and Conical Intersections. IV: A perturbative determination of the electronic energies, derivative couplings and a rigorous diabatic representation near a conical intersection. The general case*
S. Matsika and D. R. Yarkony, *J. Phys. Chem B.* **106** 8108-8116 (2002)
148. *Conical intersections and Non adiabatic Reaction $H_2O + O(^3P) \rightarrow OH(X) + OH(A)$* ;
S. Matsika and D. R. Yarkony, *J. Chem. Phys.* , **117**, 3733-3740 (2002).
147. *Photodissociation of the Hydroxymethyl Radical I. The Role of Conical Intersections in Line Broadening and Decomposition Pathway*
Brian C. Hoffman and David R. Yarkony, *J. Chem. Phys.* **116** 8300-8306, (2002).
146. *Intersecting Conical Intersection Seams: their location, representation and effect on local topography*
S. Matsika and D. R. Yarkony, *J. Phys. Chem. A.* , **106** 2580-2591 (2002).
145. *Spin-Orbit Coupling and Conical Intersection Seams in Molecules with an Odd Number of Electrons. III: A perturbative determination of the electronic energies, derivative couplings and a rigorous diabatic representation near a conical intersection*;
S. Matsika and D. R. Yarkony, *J. Chem. Phys.* , **116**, 2825 (2002).
144. *Conical intersections: The New Conventional Wisdom – Feature Article*,
D. R. Yarkony, *J. Phys. Chem. A* **105**, 6277-6293 (2001).
143. *Accurate first derivative couplings for the H_3 system*
Ravinder Abrol, Amy Shaw, Aron Kupperman and David R. Yarkony, *J. Chem. Phys.* **115**, 4640-4659, (2001)
142. *On the Effects of Spin-Orbit Coupling on Conical Intersection Seams in Molecules with an Odd Number of Electrons. II: Characterizing the local topography of the seam*
Spiridoula Matsika and David R. Yarkony, *J. Chem. Phys.* **115**, 5066-5075, (2001)
141. *On the Effects of Spin-Orbit Coupling on Conical Intersection Seams in Molecules with an Odd Number of Electrons. I: Locating the Seam*
Spiridoula Matsika and David R. Yarkony, *J. Chem. Phys.* **115**, 2038-2050 (2001)
140. *Intersecting Conical Intersection Seams in Tetra atomic Molecules : The $S_1 - S_0$ Internal Conversion in HNCO*
David R. Yarkony, *Molec Phys.* **99**, 1463-1467 (2001).
139. *Symmetry Friend or Foe: Confluences of Conical Intersection Seams in Tetraatomic Molecules*
David R. Yarkony, *J. Phys. Chem. A* **105**, 2642-2645 (2001)

138. *Nuclear Dynamics near conical intersections in the adiabatic representation: I. The effects of local topography on interstate transition*
David R. Yarkony, *J.Chem. Phys.*, 114, 2601-2613 (2001)
137. *Characterizing the Local Topology of Conical Intersections Using Orthogonality Constrained Parameters: Application to the internal conversion $S_1 \rightarrow S_0$ in HNCO*
David R. Yarkony, *J. Chem.Phys.* 114, 2614 (2001)
136. The geometric phase effect. Perspective on: *Some Recent Developments in the Theory of Molecular Energy Levels*: by H. C. Longuet-Higgins [Advances in Spectroscopy 2, 429-472 (1961)].
David R. Yarkony, *Theoretical Chemistry Accts*, New century issue, 103, 242-246 (2000).
135. *Vibronic Energies and the breakdown of the Born-Oppenheimer approximation in diatomic molecules: Adiabatic and Diabatic representations*
David R. Yarkony, in *Computational Molecular Spectroscopy*; Jensen, P. ;Bunker, P., Eds.; J. Wiley, Chichester, 2000; p. 459-484.
134. *The Role of Conical Intersections in the Non-adiabatic Quenching of OH ($A^2\Sigma^+$) by Molecular Hydrogen*
Brian C. Hoffman and David R. Yarkony, *J.Chem. Phys.*, 113, 10091(2000)
133. *On the adiabatic to diabatic states transformation near intersections of conical intersections* David R. Yarkony, *J. Chem. Phys.*, 112, 2111-2120 (2000).
- *132. *Substituent effects and the noncrossing rule: The importance of reduced symmetry subspaces. I. The quenching of OH($A^2\Sigma^+$) by H₂*
David R. Yarkony, *J. Chem. Phys.* 111, 6661-6664, (1999).
131. *Diabatic Bases and Molecular Properties*
Kryachko, E. S.; Yarkony, D. R. *Int. J. Quant. Chem.* 76, 235-243(2000).
Volume honoring Klaus Ruedenberg
130. *On the $S_1 - S_0$ Internal Conversion in Ketene: I. The Role of Conical Intersections*
David R. Yarkony, *J. Phys. Chem. A.* 103, 6658-6668 (1999).
129. *Suppressing the geometric phase effect : Closely spaced seams of conical intersection in $Na_3(2^2E')$*
David R. Yarkony *J. Chem. Phys.* 111, 4906-4912 (1999).
128. *On the Strongly Bound $B^3\Pi$ State of the CAr van der Waals Complex: Bonding and Predissociation*
Karl Sohlberg and David R. Yarkony, *J. Chem. Phys.* 111, 3070-3076 (1999).
- *127. *Unusual Conical Intersections in the Jahn-Teller Effect: The Electronically Excited States of Li₃,*
Rovshan. G. Sadygov and David. R. Yarkony, *J. Chem. Phys.* 110, 3639-3642 (1999).

126. *On the Quenching of Li (2P) by H_2 : Potential Energy Surfaces, Conical Intersection Seam, and Diabatic Bases*
Eugene S. Kryachko and David R. Yarkony, *Theoretical Chemistry Accounts*, **100**, 154 (1998)
volume in honor of Wilfred Meyer,
125. *Determining the Molecular Aharonov-Bohm phase angle: A rigorous approach employing a molecular properties based adiabatic to diabatic states transformation*
David R. Yarkony, *J. Chem. Phys.* **110**, 701-705 (1999).
124. *A theoretical analysis of the state-specific decomposition of $OH(A^2\Sigma^+, v', N', F_1 / F_2)$ levels, including the effects of spin-orbit and Coriolis interactions*
G rard Parlant and David R. Yarkony, *J. Chem. Phys.* **110**, 363-376 (1999).
123. *Conical Intersection Diabolical and Often Misunderstood*, solicited article
David R. Yarkony, *Accounts of Chemical Research*, 31, 511-518 (1998).
122. *Nonadiabatic Derivative Couplings*
David R. Yarkony, in *Encyclopedia of Computational Chemistry*, Schleyer, P. v. R.; Allinger, N. L.; Clark, T.; Gasteiger, J.; Kollman, P. A.; Schaefer III, H. F.; Schreiner, P. R., Eds.; John Wiley & Sons, Chichester, 1998.
- *121. *On the construction of diabatic bases using molecular properties. Rigorous results in the vicinity of a conical intersection*
D. R. Yarkony, *J. Phys. Chem. A* **102**, 8073-8077 (1998).
- *120. *Unanticipated Confluences of Seams of Conical Intersection. Reinvestigating intersecting potential energy surfaces using new tools, I. $C(^3P) + H_2$*
David R. Yarkony, *J. Chem. Phys.*, 109, 7047-7050, (1998)
119. *On the mechanism of the spin-nonconserving chemical reaction $O(^3P) + HCCH \rightarrow CH_2(\tilde{a} \ ^1A_1) + CO(X^1\Sigma^+)$. I. Feasibility*
David R. Yarkony, *J. Phys. Chem. A*, 102, 5305-5311(1998)
- *118. *On the Adiabatic to Diabatic States Transformation in the Presence of a Conical Intersection: A Most Diabatic Basis from the Solution to a Poisson's Equation*, Rovshan G. Sadygov and David R. Yarkony, *J. Chem. Phys.* **109**, 20-25 (1998)
117. *Systematic Location of Intersecting Seams of Conical Intersection in Triatomic Molecules: The $1^2A' - 2^2A'$ Conical Intersections in BH_2* ,
Mark S. Gordon, Vassiliki-Alexandra Glezakou, and David R. Yarkony. *J. Chem. Phys.*, **108**, 5657-5659 (1998)

116. *A compact representation of the energies and derivative couplings and locally diabatic bases for the HOH and OHH portions of the $1^1A'$ - $2^1A'$ seam of conical intersection in water,*
David R. Yarkony, *Molec. Phys.* **93**, 971-983 (1998)
115. *A Criterion for the Confluence of Two Seams of Conical Intersection in Triatomic Molecules*
David R. Yarkony, *Theoretical Chemistry Accounts*, **98**, 197-201 (1998)
114. *On the Relation Between the Bonding and the Spin-Orbit Interaction in BNe: The $C^2\Delta$ and $1^4\Pi$ States*
Karl Sohlberg and David R. Yarkony, *J. Phys. Chem. A* **101**, 9520-9524 (1997)
113. *Energies and Derivative Couplings in the Vicinity of a Conical Intersection. III The 'Most' Diabatic Basis*
Nikita Matsunaga and David R. Yarkony, *Molec. Phys.*, **93**, 79-84 (1998)
112. *On the Origin of the Heavy Atom Effect in the Fine Structure Splitting of the $1^2\Pi$ State of Alkali Metal 2P - Rare Gas van der Waals Molecules*
Karl Sohlberg and David R. Yarkony, *J. Chem. Phys.* **107**, 7690-7694 (1997)
111. *Electronic Structure Aspects of the Spin-Forbidden Reaction $CH_3(^2A_2'') + N(^4S) \rightarrow HCN(X^1\Sigma^+) + H_2(X^1\Sigma_g^+)$*
Rovshan G. Sadygov and David R. Yarkony, *J. Chem. Phys.* **107**, 4994-4999, (1997)
110. *The reactions $Al(^2P) + H_2 \rightarrow AlH_2(1^2A', 2^2A') \rightarrow AlH_2(X^2A_1)$ or $AlH(X^1\Sigma^+) + H$, Unusual Conical intersections and possible nonadiabatic recrossing*
Galina Chaban, Mark S. Gordon and David R. Yarkony *J. Phys. Chem. A* **101**, 7953-7959 (1997)
109. *Energies and Derivative Couplings in the Vicinity of a Conical Intersection. II: $CH_2(2^3A'', 3^3A'')$ and $H_2S(1^1A'', 2^1A'')$, Unexpected Results in an Ostensibly Standard Case*
Nikita Matsunaga and David R. Yarkony, *J. Chem. Phys.* **107**, 7825-7838 (1997)
108. *Energies and Derivative Couplings in the Vicinity of a Conical Intersection using Degenerate Perturbation Theory and Analytic Gradient Techniques,*
David R. Yarkony, *J. Phys. Chem. A*, **101**, 4263 (1997)
107. *A Theoretical Investigation of the Spin-Orbit Induced Predissociation of BAr $C^2\Delta$*
Karl Sohlberg and David R. Yarkony, *J. Chem. Phys.* **106**, 6607-6611 (1997).
106. *New and unusual bonding in open-shell van der Waals molecules revealed by the heavy atom effect: The case of BAr*
Karl Sohlberg and David R. Yarkony, *J. Phys. Chem. A*, 3166-3173, (1997)
105. *Resonances in the Predissociation of the $A^2\Pi_Q$ State of MgBr*
Rovshan G. Sadygov, Joëlle Rostas, Guy Taieb and David R. Yarkony. *J. Chem. Phys.* **106**, 4091-4101 (1997).
104. *Current Issues in Nonadiabatic Chemistry – Feature Article,*

- D. R. Yarkony J. Phys. Chem. **100**, 18612 (1996)
103. *Diabolical Conical Intersections*
D. R. Yarkony, Rev. Mod. Phys. **68**, 985 (1996)
102. *Molecular structure*
D. R. Yarkony, in Atomic, Molecular and Optical Physics Handbook , G. F. Drake, editor (AIP, 1996)
101. *On the Consequences of Nonremovable Derivative Couplings, I. The Geometric Phase and Quasi-Adiabatic States: A Numerical Study*
David R. Yarkony, J. Chem. Phys. **105**, 10456 (1996)
100. *On the Quenching of $CH(a^4\Sigma^-)$ by $CO(X^1\Sigma^+)$: Surfaces of Intersection, Spin-orbit Interactions and the Incorporation of Kramers' Degeneracy*
David R. Yarkony, J. Phys. Chem. **100**, 17439, (1996)
99. *On the Role of Conical Intersections in Photodissociation: V Conical Intersections and the Geometric Phase in the Photodissociation of Methyl Mercaptan*
David R. Yarkony, J. Chem. Phys. **104**, 7866(1996)
98. *Radiative and Nonradiative Decay of the $BH(b^3\Sigma^-)$ State: A Joint Experimental and Theoretical Study*
Xin Yang, Lisa Pederson, David R. Yarkony, and Paul J. Dagdigian, J. Phys. Chem. **100**, 5649 (1996)
97. *On the Role of Conical Intersections in Photodissociation: IV. Conical Intersections and the Geometric Phase in the $2^3A''$ and $3^3A''$ States of CH_2*
David R. Yarkony, J. Chem. Phys. **104**, 2932(1996)
96. *Radiative and Radiationless Decay of Multichannel Resonances Resulting from Electronically Nonadiabatic Interactions: A Computational Approach Valid for both Narrow and Broad Linewidths and Large Energy Shifts*
Seungsuk Han and David R. Yarkony, Molec Phys. **88**,53 (1996)
95. *Electronic Structure Aspects of Nonadiabatic Processes in Polyatomic Systems*
D. R. Yarkony, in Modern Electronic Structure Theory, ed.. D. R. Yarkony (World Scientific, Singapore, 1995).
94. *On the Structure and Stability of Geometrical Isomers of N_3F*
Galina Chaban, David R. Yarkony, Mark S. Gordon, J. Chem. Phys. **103**, 7983(1995).
93. *Radiative and Radiationless Decay of Resonances Resulting from Electronically Nonadiabatic Interactions: A Computational Approach Valid for both Narrow and Broad Linewidths and Large Energy Shifts*
Seungsuk Han and David R. Yarkony , J. Chem. Phys. **103**, 7336 (1995)

92. *On the role of conical intersections in photodissociation III: The case of hydroxylamine*,
Hinne Hettema and David R. Yarkony, J. Chem. Phys. **102**, 8431 (1995)
91. *On the Spin-orbit induced Radiationless Decay of the $b^3\Sigma^-$ State of BH*
Lisa A. Pederson and David R. Yarkony, Mol. Phys. **84**,611(1995).
90. *Radiationless Decay of the $1,2,3^3\Pi_g$ States of Al_2 : A Fully First Principles Treatment using
Adiabatic and Rigorous Diabatic States*
Seungsuk Han, Hinne Hettema and David R. Yarkony, J. Chem. Phys. **102**, 1955 (1995)
89. *On the Role of Conical Intersections of Two Potential Energy Surfaces of the Same
Symmetry in Photodissociation. II. $CH_3SCH_3 \rightarrow CH_3S + CH_3$*
M. Riad Manaa and David R. Yarkony, J. Amer. Chem. Soc., **116**, 11444 (1994).
88. *A Theoretical Treatment of the Radiative Decay of the ($a^3\Pi, v, N, F_i, e/f$) Levels of BH*
Lisa Pederson, Hinne Hettema and David Yarkony, J. Phys. Chem. **98**, 11069 (1994).
87. *On the Radiative Lifetime of the ($a^4\Sigma^-, v, N, F_i$) Levels of the CH Radical: An Ab Initio
Treatment*
Hinne Hettema and David R. Yarkony, J. Chem. Phys. **100**,8991(1994)
86. *Nonadiabatic Perturbations and Fine Structure Splittings in the $1,2^3\Pi_g$ States of B_2 : An
Analysis Based on Adiabatic and Rigorous Diabatic States*
M. Riad Manaa and David R. Yarkony J. Chem. Phys. **100**, 8204 (1994)
85. *On the Role of Conical Intersections of Two Potential Energy Surfaces of the Same
Symmetry in Photodissociation. I. $CH_3SH \rightarrow CH_3S + H$ and $CH_3 + SH$*
David R. Yarkony, J. Chem. Phys. **100**, 3639 (1994)
84. *On the Perturbation of the \tilde{B}^2A' State of HCO by the $1^4A''$ and $1^4A'$ States: Surfaces of
Intersection and Spin-orbit Interactions*
M. Riad Manaa and David R. Yarkony, J. Chem. Phys. **100**, 473 (1994).
83. *On the Intersection of Two Potential Energy Surfaces of the Same Symmetry: Systematic
Characterization Using a Lagrange Multiplier Constrained Procedure*
M. Riad Manaa and David R. Yarkony, J. Chem. Phys. **99**, 5251 (1993).
82. *On the Electronic Structure Aspects of Spin-Forbidden Processes in N_2O*
Agnes H. H. Chang and David R. Yarkony, J. Chem. Phys. **99**, 6824 (1993).
81. *Systematic Determination of Intersections of Potential Energy Surfaces Using a Lagrange
Multiplier Constrained Procedure*
David R. Yarkony, J. Phys. Chem. **97**, 4407 (1993)
80. *Avoided Surface Crossings and Nonadiabatic Effects in the Electronic Quenching Reaction
 $Li(^2P) + HCl \rightarrow LiCl + H(^2S)$*
M. Riad Manaa and David R. Yarkony, J. Phys. Chem. **97**, 4989 (1993).

79. *Theoretical Studies of Spin-Forbidden Radiationless Decay in Polyatomic Systems II: Radiationless Decay of α -N₂O₂*
Kiet A. Nguyen, Mark S. Gordon, John A. Montgomery, Jr., H. Harvey Michels and David R. Yarkony, *J. Chem. Phys.* **98**, 3845 (1993)
78. *On the Spin-Forbidden Predissociation of the Ro-vibronic Levels of OH⁺($c^1\Pi$)*
David R. Yarkony, *J. Phys. Chem.*, **97**, 111 (1993).
77. *Spin-forbidden Chemistry Within the Breit-Pauli Approximation*
D. R. Yarkony, *Int. Reviews of Phys. Chem.* **11**, 195 (1992).
76. *Nonadiabatic Interactions Between Potential Energy Surfaces: Theory and Applications*
B. H. Lengsfeld and D. R. Yarkony, *Advances in Chemical Physics: State-Selected and State to State Ion-Molecule Reaction Dynamics: Theory, Part II*, eds. C. Y. Ng and M. Baer, (John Wiley and Sons, New York, 1992), vol 82.
75. *On the Intersection of Potential Energy Surfaces in Charge Transfer Reactions: A Crossing Seam for Two States of the Same Symmetry in the Reaction $H^+ + NO(X^2\Pi) \rightarrow H + NO^+(X^1\Sigma^+)$*
M. R. Manaa and D. R. Yarkony, *J. Chem. Phys.*, **97**, 715 (1992).
74. *An Adiabatic State Approach to Electronically Nonadiabatic WavePacket Dynamics*
G. Parlant and D. R. Yarkony, *Int. J. Quantum Chem.*, **S26**, 737-739, (1992).
73. *A Theoretical Treatment of the Predissociation on the Individual Rovibronic Levels of OH/OD($A^2\Sigma^+$)*
D. R. Yarkony, *J. Chem. Phys.* **97**, 1838 (1992).
72. *Theoretical Studies of Spin-Forbidden Radiationless Decay in Polyatomic Systems: Insights from Recently Developed Computational Methods*
David R. Yarkony, *J. Amer. Chem. Soc.*, **114**, 5406, (1992)
71. *Predissociation of the NH/ND($c^1\Pi, v'J'$) States*
B. Bohn, F. Stuhl, G. Parlant, P. J. Dagdigian, and D. R. Yarkony, *J. Chem. Phys.*, **96**, 5059 (1992).
70. *On the Mechanism of the Reaction $CH(X^2\Pi) + N_2(X^1\Sigma_g^+) \rightarrow HCN(X^1\Sigma^+) + N(^4S)$. II: The Intermediate Complex Region*
M. Riad Manaa and David R. Yarkony, *Chem. Phys. Lett.*, **188**, 352 (1992).
69. *A Theoretical Treatment of the $a^3\Sigma_1^+ \rightarrow X^1\Sigma_{0^+}^+$ Spin-Forbidden Dipole-Allowed Radiative Transition in NO⁺*
M. Riad Manaa and David R. Yarkony, *J. Chem. Phys.*, **95**, 6562 (1991)
68. *On the Mechanism of the Reaction $CH(X^2\Pi) + N_2(X^1\Sigma_g^+) \rightarrow HCN(X^1\Sigma^+) + N(^4S)$. I: A Theoretical Treatment of the Electronic Structure Aspects of the Intersystem Crossing*
M. Riad Manaa and David R. Yarkony, *J. Chem. Phys.*, **95**, 1808 (1991)

67. *Spin-Forbidden Decay of the Dication HS^{2+}*
Gérard Parlant, Jörg Senekowitsch, Stephen V. O'Neil, David R. Yarkony, J. Chem. Phys., 94, 7208 (1991).
66. *Predissociation of the $c^1\Pi$ state of $NH(ND)$: The role of dipolar spin-spin coupling.*
Gérard Parlant, Paul J. Dagdigian and David R. Yarkony, J. Chem. Phys., 94, 2364 (1991).
65. *Radiative and Nonradiative Decay of the $NH(ND) A^3\Pi$ Electronic State: Predissociation Induced by the $^5\Sigma^-$ State*
Dipti Patel-Misra, Gérard Parlant, Deborah G. Sauder, David R. Yarkony and Paul J. Dagdigian, J. Chem. Phys., 94, 1913 (1991).
64. *On the Electronic Structure and Dynamical Aspects of the Predissociation of the $A^2\Pi_Q$ States of $MgCl$. A Rigorous Quantum Mechanical Treatment Incorporating Spin-Orbit and Derivative Coupling Effects.*
Gérard Parlant, Joëlle Rostas, Guy Taieb and David R. Yarkony, J. Chem. Phys., 93, 6403 (1990)
63. *On the Noncrossing Rule in Polyatomic Systems: Determination of a Seam of Actual Surface Crossings Relevant to the Quenching of $H_2(B^1\Sigma_u^+)$ by Helium*
M. R. Manaa and D. R. Yarkony, J. Chem. Phys. 93, 4473 (1990)
62. *Theoretical Studies of the Electronic Structure Aspects of Electronically Nonadiabatic Processes Using Analytic Gradient Techniques: Seams of Avoided Crossings in the Electronic Quenching Reaction $Na(^2P) + HCl \rightarrow NaCl + H(^2S)$*
D. R. Yarkony, J. Phys. Chem. 94, 5572 (1990)
Proceedings of "Forty Years of Quantum Chemistry", Oct. 1989
61. *Spin-Orbit Effects in the Decomposition Reaction $N_3H(X^1A') \rightarrow N_2(X^1\Sigma_g^+) + NH(X^3\Sigma, a^1\Delta)$*
D. R. Yarkony, J. Chem. Phys., 92, 320 (1990).
60. *On the Characterization of Regions of Avoided Surface Crossings Using an Analytic Gradient Based Method*
D. R. Yarkony, J. Chem. Phys., 92, 2457 (1990).
59. *On the Electronic Structure of the NH Radical. The Fine Structure Splitting of the $X^3\Sigma^-$ State and the Spin-Forbidden $(b^1\Sigma^+, a^1\Delta) \rightarrow X^3\Sigma^-$, and the Spin-Allowed $A^3\Pi \rightarrow X^3\Sigma^-$ and $c^1\Pi \rightarrow (b^1\Sigma^+, a^1\Delta)$ Radiative Transitions.*
D. R. Yarkony, J. Chem. Phys., 91, 4745 (1989).
58. *On the Quenching of Helium 2^3S : Potential Energy Curves for, and Nonadiabatic, Relativistic and Radiative Couplings Between, the $a^3\Sigma_u^-$, $A^1\Sigma_u^-$, $b^3\Pi_g$, $B^1\Pi_g$, $c^3\Sigma_g^-$ and $C^1\Sigma_g^+$ States of He_2 .*
D. R. Yarkony, J. Chem. Phys. 90, 7164 (1989).
57. *Theoretical Study of the Radiative Lifetime for the Spin-Forbidden Transition $X^1\Sigma_g^+ \leftarrow a^3\Sigma_u^+$ in He_2 .*

- C. F. Chabalowski, J. O. Jensen, D. R. Yarkony and B. H. Lengsfeld, *J. Chem. Phys.*, **90**, 2504(1989).
56. *Nonadiabatic Effects in the Vicinity of Multiple Surface Crossings. Evaluation of Derivative Couplings with Respect to Rotational and Internal Degrees of Freedom. Application to the Charge Transfer Reaction: $H^+ + NO \rightarrow H + NO^+$.*
D. R. Yarkony, *J. Chem. Phys.*, **90**, 1657 (1989).
 55. *Spin-Forbidden Radiative Decay Involving Quasi Degenerate States. Application to the $B^1\Sigma^+ \rightarrow a^3\Pi$ Transition in MgO.*
D. R. Yarkony, *J. Chem. Phys.*, **89**, 7324 (1988).
 54. *On the Electronic Structure of the He^-H_2 System Characterization of, and Nonadiabatic Interactions Between, the $1^1A'$ and $2^1A'$ Potential Energy Surfaces.*
J. K. Perry and D. R. Yarkony, *J. Chem. Phys.*, **89**, 4945 (1988).
 53. *On the Evaluation of Non Born-Oppenheimer Interactions for Born-Oppenheimer Wavefunctions V: A Body Fixed Frame Approach. Applications to Isotope Effects of Equilibrium Geometries and the Adiabatic Correction for the $X^1\Sigma^+$ State of LiH.*
J. O. Jensen and D. R. Yarkony, *J. Chem. Phys.*, **89**, 975 (1988).
 52. *On the Evaluation of Lifetimes for Spin-Forbidden Radiative Transitions Originating in Coupling to States Embedded in a Continuum. Application to CH^- .*
B. H. Lengsfeld, J. O. Jensen, and D. R. Yarkony, *J. Chem. Phys.* **88**, 3853 (1988).
 51. *On the Characterization of the Dipolar Spin-Spin Interaction in Molecular Systems: A Symbolic Matrix Element Approach.*
J. O. Jensen and D. R. Yarkony, *Chem. Phys. Lett.* **141**, 391 (1987).
 50. *On the Quenching of Na (2P) by HCl: Nonadiabatic Effects.*
M. M. Gallo and D. R. Yarkony, *J. Chem. Phys.*, **86**, 4990 (1987).
 49. *On the Radiative Lifetimes of the $b^1\Sigma^+$ and $a^1\Delta$ States in NCl.*
D. R. Yarkony, *J. Chem. Phys.*, **86**, 1642 (1987).
 48. *A Theoretical Description of the Radiative Decay Processes ($b^1\Sigma^+$, $a^1\Delta$) $\rightarrow X^3\Sigma^-$ in NF.*
D. R. Yarkony, *J. Chem. Phys.*, **85**, 7261 (1986).
 47. *On the Evaluation of Nonadiabatic Coupling Matrix Elements for MCSCF/CI Wavefunctions IV. Second Derivative Terms Using Analytic Gradient Methods.*
P. Saxe and D. R. Yarkony, *J. Chem. Phys.*, **86**, 321 (1987).
 46. *On the Quenching of Li (2P) by HCl: Nonadiabatic Effects.*
D. R. Yarkony, *Int'l. J. Quant. Chem.* **31**, 91 (1987).
 45. *On the Reaction $Na(^2P) + H_2 \rightarrow Na(^2S) + H_2$ Nonadiabatic Effects.*
D. R. Yarkony, *J. Chem. Phys.* **84**, 3206 (1986).
 44. *On the Use of the Breit-Pauli Approximation for Evaluating Line Strengths for Spin-Forbidden Transitions II: The Symbolic Matrix Element Method.*
D. R. Yarkony, *J. Chem. Phys.* **84**, 2075 (1986).

43. *On the Evaluation of Nonadiabatic Coupling Matrix Elements for MCSCF/CI Wavefunctions Using Analytic Derivative Methods III. Second Derivative Terms.*
B. H. Lengsfeld and D. R. Yarkony, J. Chem. Phys. 84, 348 (1986).
42. *On the Use of the Breit-Pauli Approximation for Evaluating Line Strengths for Spin-Forbidden Transitions. Application to NF.*
S. J. Havriliak and D. R. Yarkony, J. Chem. Phys. 83, 1168 (1985).
41. *On the Reaction $\text{Ca}(^1S) + \text{Cl}_2(^1\Sigma_g^+) \rightarrow \text{CaCl}(X^2\Sigma^+) + \text{Cl}(^2P)$.*
N. Honjou and D. R. Yarkony, J. Phys. Chem. 89, 2919 (1985).
40. *On the Evaluation of Nonadiabatic Coupling Matrix Elements for Large Scale CI-Wavefunctions.*
P. Saxe, B. H. Lengsfeld, and D. R. Yarkony, Chem. Phys. Lett. 113, 159 (1985).
39. *The Electronic Structure of the Low-Lying $^2\Sigma^+$ and $^2\Pi$ Valence States of CO^+ .*
N. Honjou and D. R. Yarkony, J. Phys. Chem. 89, 44 (1985).
38. *On the Evaluation of Nonadiabatic Coupling Matrix Elements Using SA-MCSCF/CI Wavefunctions and Analytic Gradient Methods. I*
B. H. Lengsfeld, P. Saxe, and D. R. Yarkony, J. Chem. Phys. 81, 4549 (1984).
37. *On the $\text{Mg}(^3P)\text{-He}(^1S)$ Interaction Using SA-MCSCF/ICF-CI Wavefunctions.*
B. Pouilly, B. H. Lengsfeld, and D. R. Yarkony, J. Chem. Phys. 80, 5089 (1984).
36. *On the Electronic Structure of the X, A and B States of CaCl .*
N. Honjou, G. F. Adams and D. R. Yarkony, J. Chem. Phys. 79, 4376 (1983).
35. *On the Reaction: $\text{Mg} + \text{N}_2\text{O} \rightarrow \text{MgO} + \text{N}_2$.*
D. R. Yarkony, J. Chem. Phys. 78, 6763 (1983).
34. *The Electronic Structure of CaO II : An MCSCF/CI Treatment of the Low-Lying $^1\Sigma^+$ and $^1\Pi$ States.*
R. N. Diffenderfer and D. R. Yarkony, J. Chem. Phys. 77, 5573 (1982).
33. *The Electronic Structure and Vertical Excitation Spectrum of Methylene Amidogen, CH_2N .*
G. F. Adams, D. R. Yarkony, R. J. Bartlett, and G. D. Purvis, Int'l. J. of Quant. Chem. 23, 437 (1983).
32. *Radiative Lifetimes and Transition Moments in MgO .*
R. N. Diffenderfer, D. R. Yarkony and P. J. Dagdigian, J. Quant. Spectr. and Rad. Trans. 29, 329 (1983).
31. *Use of the State Averaged-MCSCF Procedure: Application to Radiative Transitions in MgO .*
R. N. Diffenderfer and D. R. Yarkony, J. Phys. Chem. 86, 5098 (1982).
30. *Multiconfiguration Self Consistent Field Wave functions for Excited States*
C. W. Bauschlicher, D. M. Silver and D. R. Yarkony, in Lecture Notes in Chemistry : The Unitary Group, ed. J. Hinze, (Springer-Verlag, Heidelberg, 1981), vol 22.

29. *On the Low-Lying States of MgO: II.*
C. W. Bauschlicher, Jr., B. H. Lengsfeld, D. M. Silver and D. R. Yarkony, *J. Chem. Phys.* **74**, 2379 (1981).
28. *A Hybrid Method Improving MCSCF Convergence.*
C. W. Bauschlicher, Jr., P. S. Bagus, D. R. Yarkony and B. H. Lengsfeld, *J. Chem. Phys.* **74**, 3965 (1981).
27. *Comment on the Use of the Augmented Matrix in MCSCF Theory.*
D. R. Yarkony, *Chem. Phys. Lett.* **77**, 634 (1981).
26. *On the Low-Lying Singlet States of BeO.*
C. W. Bauschlicher, Jr., B. H. Lengsfeld and D. R. Yarkony, *J. Chem. Phys.* **73**, 5702 (1980).
25. Spin Forbidden Radiative Transitions in Atomic Calcium.
R. N. Diffenderfer, P. J. Dagdigian and D. R. Yarkony, *J. Phys. B.* **14**, 21 (1981).
24. The Electronic Structure of Polydiacetylenes: Cyclic vs Linear Models.
K. Balasubramanian and D. R. Yarkony, *Chem. Phys. Lett.* **70**, 374 (1980).
23. An SCF and MCSCF Description of the Low-Lying States of MgO.
C. W. Bauschlicher, D. M. Silver and D. R. Yarkony, *J. Chem. Phys.* **73**, 2867 (1980).
22. A Genealogical Electronic Coupling Procedure Incorporating the Hartree-Fock Interacting Space and Suitable for Degenerate Point Groups: Application to Excited States of BH₃.
W. C. Swope, H. F. Schaefer and D. R. Yarkony, *J. Chem. Phys.* **73**, 407 (1980).
21. Experimental and Theoretical Study of the Ca I 4s3d ¹D – 4s ¹S and 4s4p ³P₁ – 4s² ¹S Forbidden Transitions.
L. Pasternack, D. M. Silver, D. R. Yarkony and P. J. Dagdigian, *J. Phys. B.* **13**, 2231 (1980).
20. MCSCF Wavefunctions for Excited States of Polar Molecules: Applications to BeO.
C. W. Bauschlicher and D. R. Yarkony, *J. Chem. Phys.* **72**, 1138 (1980).
19. On the Electronic Structure of the 2 ¹A₁ State of Methylene.
C. W. Bauschlicher and D. R. Yarkony, *J. Chem. Phys.* **69**, 3875 (1978).
18. Comment on the Electronic Structure of Polydiacetylenes.
D. R. Yarkony, *Chem. Phys.* **33**, 171 (1978).
17. Electronic Structure of CaO: I.
C. W. Bauschlicher, Jr. and D. R. Yarkony, *J. Chem. Phys.* **68**, 3990 (1978).
16. Comment on Polaritons in a Spatially Dispersive Medium: Surface Effects I.

- D. R. Yarkony and R. Silbey, *Phys. Rev. B.* *17*, 2420 (1978).
15. Symmetry Restricted Multiconfiguration Annihilation of Single Excitations II: Applications: Electronic States of Methyl Nitrene.
R. R. Lucchese and D. R. Yarkony, *J. Chem. Phys.* *68*, 2696 (1978).
 14. Variational Approach to Exciton Transport in Molecular Crystals.
D. R. Yarkony and R. Silbey, *J. Chem. Phys.* *67*, 5818 (1977).
 13. Symmetry-Adapted-Multiconfiguration SCF Wavefunctions via Symmetry-Restricted Annihilation of Single Excitations: I.
D. R. Yarkony, *J. Chem. Phys.* *66*, 2045 (1977).
 12. The Band Gap in Linear Polyenes.
D. R. Yarkony and R. Silbey, *Chem. Phys.* *20*, 183 (1977).
 11. Comment on Exciton-Phonon Coupling: Temperature Dependence.
D. R. Yarkony and R. Silbey, *J. Chem. Phys.* *65*, 1042 (1976).
 10. Self-Consistent-Field Wavefunctions using a Symmetry-Restricted Annihilation of Single-Excitations Procedure.
D. R. Yarkony, H. F. Schaefer and C. F. Bender, *J. Chem. Phys.* *64*, 981 (1976).
 9. The Acetyl Cation and its Geometrical Isomers.
D. R. Yarkony and H. F. Schaefer, *J. Chem. Phys.* *63*, 4317 (1975).
 8. Multiplet Splittings in the Photoelectron Spectra of Organic Radicals: Trimethylenemethane.
D. R. Yarkony and H. F. Schaefer, *Chem. Phys. Letters* *35*, 291 (1975).
 7. Correlation Diagram for $\text{He} + \text{He} \rightarrow \text{Be}$.
D. R. Yarkony and H. F. Schaefer, *J. Chem. Phys.* *61*, 4921 (1974).
 6. X^3A_2 , a^1E and b^1A_1 Electronic States of Methyl Nitrene.
D. R. Yarkony, H. F. Schaefer and S. Rothenberg, *J. Amer. Chem. Soc.* *96*, 5974 (1974).
 5. Triplet Electronic Ground State of Trimethylenemethane.
D. R. Yarkony and H. F. Schaefer, *J. Amer. Chem. Soc.* *96*, 3754 (1974).
 4. Geometries of the Methoxy Radical (X^2E and A^2A_1 States) and the Methoxide Ion.
D. R. Yarkony, H. F. Schaefer and S. Rothenberg, *J. Amer. Chem. Soc.* *96*, 656 (1974).
 3. Interaction Potential Between Two Rigid HF Molecules.
D. R. Yarkony, S. V. O'Neil, H. F. Schaefer, C. P. Baskin and C. F. Bender, *J. Chem. Phys.* *60*, 855 (1974).

2. Relation Between Electronic Structure and the Chemiluminescence Arising from Collisions Between Alkaline Earth Atoms and Halogen Molecules.
D. R. Yarkony, W. J. Hunt, H. F. Schaefer, *Mol. Phys.* *26*, 941 (1973).
1. Walsh Diagram for Zinc Difluoride.
D. R. Yarkony and H. F. Schaefer, *Chem. Phys. Letters* *15*, 514 (1972).

*appeared/to appear, as a communication-*J. Chem. Phys* or letter –*J. Phys. Chem.*

** accepted as a communication appeared as a regular article owing to its length