David R Yarkony

List of Publications by Citations

201 papers	8,911 citations	43 h-index	85 g-index
209 ext. papers	9,465 ext. citations	4.9 avg, IF	6.74 L-index

#	Paper	IF	Citations
201	Diabolical conical intersections. *Reviews of Modern Physics*, **1996**, 68, 985-1013	40.5	735
200	Conical Intersections. *Advanced Series in Physical Chemistry*, **2004**,		679
199	Conical Intersections: Diabolical and Often Misunderstood. *Accounts of Chemical Research*, **1998**, 31, 511-518	24.3	364
198	Role of conical intersections in molecular spectroscopy and photoinduced chemical dynamics. *Annual Review of Physical Chemistry*, **2012**, 63, 325-52	15.7	332
197	Conical Intersections:The New Conventional Wisdom. *Journal of Physical Chemistry A*, **2001**, 105, 6277-6293	2.8	300
196	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. I. Formalism. *Journal of Chemical Physics*, **2004**, 120, 7322-9	3.9	270
195	Conical Intersections. *Advanced Series in Physical Chemistry*, **2011**,		233
194	Analytic evaluation of nonadiabatic coupling terms at the MR-CI level. II. Minima on the crossing seam: formaldehyde and the photodimerization of ethylene. *Journal of Chemical Physics*, **2004**, 120, 7330-9	3.9	208
193	Nonadiabatic quantum chemistry--past, present, and future. *Chemical Reviews*, **2012**, 112, 481-98	68.1	205
192	Current Issues in Nonadiabatic Chemistry *The Journal of Physical Chemistry*, **1996**, 100, 18612-18628		166
191	On the evaluation of nonadiabatic coupling matrix elements using SA-MCSCF/CI wave functions and analytic gradient methods. I. *Journal of Chemical Physics*, **1984**, 81, 4549-4553	3.9	143
190	Nuclear dynamics near conical intersections in the adiabatic representation: I. The effects of local topography on interstate transitions. *Journal of Chemical Physics*, **2001**, 114, 2601-2613	3.9	141
189	On the intersection of two potential energy surfaces of the same symmetry. Systematic characterization using a Lagrange multiplier constrained procedure. *Journal of Chemical Physics*, **1993**, 99, 5251-5256	3.9	112
188	On the consequences of nonremovable derivative couplings. I. The geometric phase and quasidiabatic states: A numerical study. *Journal of Chemical Physics*, **1996**, 105, 10456-10461	3.9	109
187	Energies and Derivative Couplings in the Vicinity of a Conical Intersection Using Degenerate Perturbation Theory and Analytic Gradient Techniques. 1. *Journal of Physical Chemistry A*, **1997**, 101, 4263-4270	2.8	106
186	Nonadiabatic Tunneling in Photodissociation of Phenol. *Journal of the American Chemical Society*, **2016**, 138, 7828-31	16.4	102
185	On the evaluation of non-adiabatic coupling matrix elements for large scale CI wavefunctions. *Chemical Physics Letters*, **1985**, 113, 159-164	2.5	91

184	On the adiabatic to diabatic states transformation near intersections of conical intersections. *Journal of Chemical Physics*, **2000**, 112, 2111-2120	3.9	90
183	On the adiabatic to diabatic states transformation in the presence of a conical intersection: A most diabatic basis from the solution to a Poisson equation. I. *Journal of Chemical Physics*, **1998**, 109, 20-25	3.9	82
182	Fitting coupled potential energy surfaces for large systems: method and construction of a 3-state representation for phenol photodissociation in the full 33 internal degrees of freedom using multireference configuration interaction determined data. *Journal of Chemical Physics*, **2014**, 140, 024112	3.9	80
181	A theoretical treatment of the predissociation of the individual rovibronic levels of OH/OD(A 2). *Journal of Chemical Physics*, **1992**, 97, 1838-1849	3.9	76
180	Accurate nonadiabatic dynamics. *Physical Chemistry Chemical Physics*, **2016**, 18, 26335-26352	3.6	75
179	Spin-forbidden chemistry within the Breit-Pauli approximation. *International Reviews in Physical Chemistry*, **1992**, 11, 195-242	7	75
178	Nonadiabatic Interactions Between Potential Energy Surfaces: Theory and Applications. *Advances in Chemical Physics*,1-71		70
177	On the mechanism of the reaction CH(X 2)+N2(X 1g)-HCN(X 1) +N(4S). I. A theoretical treatment of the electronic structure aspects of the intersystem crossing. *Journal of Chemical Physics*, **1991**, 95, 1808-1816	3.9	68
176	Beyond two-state conical intersections. Three-state conical intersections in low symmetry molecules: the allyl radical. *Journal of the American Chemical Society*, **2003**, 125, 10672-6	16.4	65
175	Toward eliminating the electronic structure bottleneck in nonadiabatic dynamics on the fly: an algorithm to fit nonlocal, quasidiabatic, coupled electronic state Hamiltonians based on ab initio electronic structure data. *Journal of Chemical Physics*, **2010**, 132, 104101	3.9	62
174	On the characterization of regions of avoided surface crossings using an analytic gradient based method. *Journal of Chemical Physics*, **1990**, 92, 2457-2463	3.9	62
173	Accidental conical intersections of three states of the same symmetry. I. Location and relevance. *Journal of Chemical Physics*, **2002**, 117, 6907-6910	3.9	60
172	Accurate first-derivative nonadiabatic couplings for the H3 system. *Journal of Chemical Physics*, **2001**, 115, 4640-4659	3.9	59
171	A theoretical analysis of the state-specific decomposition of OH(A 2,v?,N?,F1/F2) levels, including the effects of spin orbit and Coriolis interactions. *Journal of Chemical Physics*, **1999**, 110, 363-376	3.9	52
170	On the evaluation of nonadiabatic coupling matrix elements for MCSCF/CI wave functions using analytic derivative methods. III. Second derivative terms. *Journal of Chemical Physics*, **1986**, 84, 348-353	3.9	52
169	Interpolation of diabatic potential-energy surfaces: quantum dynamics on ab initio surfaces. *Journal of Chemical Physics*, **2005**, 123, 134110	3.9	50
168	On the electronic structure of the NH radical. The fine structure splitting of the X 3 state and the spin-forbidden (b 1, a 1)-X 3 and the spin-allowed A 3-X 3 and c 1-(b 1, a 1) radiative transitions. *Journal of Chemical Physics*, **1989**, 91, 4745-4757	3.9	50
167	Determining quasidiabatic coupled electronic state Hamiltonians using derivative couplings: A normal equations based method. *Journal of Chemical Physics*, **2008**, 129, 124104	3.9	48

166	Energies and derivative couplings in the vicinity of a conical intersection. II. CH2(2 3A?,3 3A?) and H2S(1 1A?,2 1A?), unexpected results in an ostensibly standard case. *Journal of Chemical Physics*, **1997**, 107, 7825-7838	3.9	47
165	Electronic structure of CaO. I. *Journal of Chemical Physics*, **1978**, 68, 3990-3997	3.9	47
164	On the reaction Mg+N2O-MgO+N2. *Journal of Chemical Physics*, **1983**, 78, 6763-6772	3.9	46
163	The Reactions Al(2P) + H2 -AlH2(12A22A)-AlH2(X2A1) or AlH(X1) + H: Unusual Conical Intersections and Possible Nonadiabatic Recrossing. *Journal of Physical Chemistry A*, **1997**, 101, 7953-7959	2.8	45
162	Conical intersections of three electronic states affect the ground state of radical species with little or no symmetry: pyrazolyl. *Journal of the American Chemical Society*, **2003**, 125, 12428-9	16.4	45
161	On the reaction Na(2P)+H2-Na(2S)+H2 nonadiabatic effects. *Journal of Chemical Physics*, **1986**, 84, 3206-3211	3.9	45
160	Full-Dimensional Quantum State-to-State Nonadiabatic Dynamics for Photodissociation of Ammonia in its A-Band. *Journal of Physical Chemistry Letters*, **2014**, 5, 1055-60	6.4	44
159	The role of conical intersections in the nonadiabatic quenching of OH(A 2) by molecular hydrogen. *Journal of Chemical Physics*, **2000**, 113, 10091-10099	3.9	44
158	On the representation of coupled adiabatic potential energy surfaces using quasi-diabatic Hamiltonians: a distributed origins expansion approach. *Journal of Chemical Physics*, **2012**, 136, 174110	3.9	43
157	Permutation invariant polynomial neural network approach to fitting potential energy surfaces. IV. Coupled diabatic potential energy matrices. *Journal of Chemical Physics*, **2018**, 149, 144107	3.9	43
156	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. *Journal of Chemical Physics*, **2012**, 137, 22A511	3.9	42
155	Computational determination of the state absorption spectrum of NH3 and of ND3 using a new quasi-diabatic representation of the X and states and full six-dimensional quantum dynamics. *Journal of Chemical Physics*, **2012**, 136, 234301	3.9	42
154	On the Construction of Diabatic Bases Using Molecular Properties. Rigorous Results in the Vicinity of a Conical Intersection. *Journal of Physical Chemistry A*, **1998**, 102, 8073-8077	2.8	42
153	On the electronic structure aspects of spin-forbidden processes in N2O. *Journal of Chemical Physics*, **1993**, 99, 6824-6831	3.9	41
152	Radiative and nonradiative decay of the NH(ND) A 3electronic state: Predissociation induced by the 5state. *Journal of Chemical Physics*, **1991**, 94, 1913-1922	3.9	41
151	On the simulation of photoelectron spectra in molecules with conical intersections and spin-orbit coupling: the vibronic spectrum of CH3S. *Journal of Chemical Physics*, **2007**, 127, 104309	3.9	40
150	CONICAL INTERSECTIONS: THEIR DESCRIPTION AND CONSEQUENCES. *Advanced Series in Physical Chemistry*, **2004**, 41-127		38
149	First principles determination of the NH2ND2(X) branching ratios for photodissociation of NH3ND3 via full-dimensional quantum dynamics based on a new quasi-diabatic representation of coupled ab initio potential energy surfaces. *Journal of Chemical Physics*, **2012**, 137, 22A541	3.9	37

148	Exploring molecular complexity: conical intersections and NH3 photodissociation. *Journal of Chemical Physics*, **2004**, 121, 628-31	3.9	37
147	Diabatic bases and molecular properties. *International Journal of Quantum Chemistry*, **2000**, 76, 235-243	2.1	37
146	On the use of the Breit□Pauli approximation for evaluating line strengths for spin-forbidden transitions: Application to NF. *Journal of Chemical Physics*, **1985**, 83, 1168-1172	3.9	37
145	Encoding of vinylidene isomerization in its anion photoelectron spectrum. *Science*, **2017**, 358, 336-339	33.3	36
144	Nonadiabatic processes involving three electronic states. I. Branch cuts and linked pairs of conical intersections. *Journal of Chemical Physics*, **2003**, 119, 5058-5068	3.9	36
143	Nonadiabatic tunneling via conical intersections and the role of the geometric phase. *Physical Review A*, **2017**, 95,	2.6	35
142	On the vibronic coupling approximation: a generally applicable approach for determining fully quadratic quasidiabatic coupled electronic state Hamiltonians. *Journal of Chemical Physics*, **2007**, 127, 094104	3.9	35
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140	On the evaluation of non-Born□Oppenheimer interactions for Born□Oppenheimer wave functions. V. A body fixed frame approach. Applications to isotope effects on equilibrium geometries and the adiabatic correction for the X 1□ state of LiH. *Journal of Chemical Physics*, **1988**, 89, 975-982	3.9	35
139	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. *Journal of Chemical Physics*, **2016**, 144, 024105	3.9	35
138	Marching along Ridges. Efficient Location of Energy-Minimized Conical Intersections of Two States Using Extrapolatable Functions. *Journal of Physical Chemistry A*, **2004**, 108, 3200-3205	2.8	34
137	Representation of coupled adiabatic potential energy surfaces using neural network based quasi-diabatic Hamiltonians: 1,2 A' states of LiFH. *Physical Chemistry Chemical Physics*, **2019**, 21, 14205-14213	3.6	34
136	An improved quasi-diabatic representation of the 1, 2, 3(1)A coupled adiabatic potential energy surfaces of phenol in the full 33 internal coordinates. *Journal of Chemical Physics*, **2016**, 144, 124312	3.9	33
135	On the quenching of helium 2 3S: Potential energy curves for, and nonadiabatic, relativistic, and radiative couplings between, the a 3□u, A 1□u, b 3□g, B 1□g, c 3□g, and C 1□g states of He2. *Journal of Chemical Physics*, **1989**, 90, 7164-7175	3.9	33
134	On the evaluation of nonadiabatic coupling matrix elements for MCSCF/CI wave functions. IV. Second derivative terms using analytic gradient methods. *Journal of Chemical Physics*, **1987**, 86, 321-328	3.9	33
133	On the electronic structure of the X, A, and B states of CaCl. *Journal of Chemical Physics*, **1983**, 79, 4376-4381	3.9	33
132	MCSCF wave functions for excited states of polar molecules: Application to BeO. *Journal of Chemical Physics*, **1980**, 72, 1138-1144	3.9	33
131	Signatures of a Conical Intersection in Adiabatic Dissociation on the Ground Electronic State. *Journal of the American Chemical Society*, **2018**, 140, 1986-1989	16.4	31

130	Non-adiabaticity: the importance of conical intersections. *Molecular Physics*, **2016**, 114, 1983-2013	1.7	31
129	On the role of conical intersections of two potential energy surfaces of the same symmetry in photodissociation. I. CH3SH-ĉH3S+H and CH3+SH. *Journal of Chemical Physics*, **1994**, 100, 3639-3644	3.9	31
128	On the low-lying states of MgO. II. *Journal of Chemical Physics*, **1981**, 74, 2379-2383	3.9	31
127	On the connectivity of seams of conical intersection: seam curvature. *Journal of Chemical Physics*, **2005**, 123, 204101	3.9	30
126	The electronic structure of CaO. II. An MCSCF/CI treatment of the low-lying 1Π and 1Σ states. *Journal of Chemical Physics*, **1982**, 77, 5573-5580	3.9	30
125	Neural network based quasi-diabatic Hamiltonians with symmetry adaptation and a correct description of conical intersections. *Journal of Chemical Physics*, **2019**, 150, 214101	3.9	29
124	Intersecting Conical Intersection Seams: Their Location, Representation, and Effect on Local Topography. *Journal of Physical Chemistry A*, **2002**, 106, 2580-2591	2.8	29
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120	Substituent effects and the noncrossing rule: The importance of reduced symmetry subspaces. I. The quenching of OH(A 2Σ) by H2. *Journal of Chemical Physics*, **1999**, 111, 6661-6664	3.9	28
119	On the noncrossing rule in polyatomic systems: Determination of a seam of actual surface crossings relevant to the quenching of H2(B 1Σu) by helium. *Journal of Chemical Physics*, **1990**, 93, 4473-4474	3.9	28
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117	Up to a Sign. The Insidious Effects of Energetically Inaccessible Conical Intersections on Unimolecular Reactions. *Accounts of Chemical Research*, **2019**, 52, 501-509	24.3	27
116	On the effects of spin-orbit coupling on conical intersection seams in molecules with an odd number of electrons. I. Locating the seam. *Journal of Chemical Physics*, **2001**, 115, 2038-2050	3.9	27
115	Extending the Representation of Multistate Coupled Potential Energy Surfaces To Include Properties Operators Using Neural Networks: Application to the 1,2A States of Ammonia. *Journal of Chemical Theory and Computation*, **2020**, 16, 302-313	6.4	27
114	Communication: On the competition between adiabatic and nonadiabatic dynamics in vibrationally mediated ammonia photodissociation in its A band. *Journal of Chemical Physics*, **2015**, 142, 091101	3.9	26
113	Systematic location of intersecting seams of conical intersection in triatomic molecules: The 1 2A?Σ 2A? conical intersections in BH2. *Journal of Chemical Physics*, **1998**, 108, 5657-5659	3.9	26

112	On the radiative lifetimes of the b 1Σ+ and a 1Δ states in NCl. *Journal of Chemical Physics*, **1987**, 86, 1642-1643	3.9	26
111	On the Construction of Property Based Diabatizations: Diabolical Singular Points. *Journal of Physical Chemistry A*, **2015**, 119, 12383-91	2.8	25
110	Full-dimensional quantum dynamics of vibrationally mediated photodissociation of NH3 and ND3 on coupled ab initio potential energy surfaces: absorption spectra and NH2(Ã(2)A1)/NH2(X (2)B1) branching ratios. *Journal of Physical Chemistry A*, **2014**, 118, 11926-34	2.8	25
109	ELECTRONIC STRUCTURE ASPECTS OF NONADIABATIC PROCESSES IN POLYATOMIC SYSTEMS. *Advanced Series in Physical Chemistry*, **1995**, 642-721		25
108	Spin–orbit effects in the decomposition reaction N3H(X 1A′)→N2(X1Σg)+NH(X3Δa1Δ). *Journal of Chemical Physics*, **1990**, 92, 320-323	3.9	25
107	On the use of the Breit–Pauli approximation for evaluating line strengths for spin-forbidden transitions. II. The symbolic matrix element method. *Journal of Chemical Physics*, **1986**, 84, 2075-2078	3.9	25
106	Spin-forbidden radiative decay involving quasidegenerate states. Application to the B 1Σ+-b 3Π transition in MgO. *Journal of Chemical Physics*, **1988**, 89, 7324-7333	3.9	25
105	A criterion for the confluence of two seams of conical intersection in triatomic molecules. *Theoretical Chemistry Accounts*, **1998**, 98, 197-201	1.9	24
104	Photodissociation of the hydroxymethyl radical. I. The role of conical intersections in line broadening and decomposition pathways. *Journal of Chemical Physics*, **2002**, 116, 8300	3.9	24
103	On the Mechanism of the Spin-Nonconserving Chemical Reaction O(3P) + HCCH →CH2(X̃1A1) + CO(X1Σ+). I. Feasibility. *Journal of Physical Chemistry A*, **1998**, 102, 5305-5311	2.8	24
102	On the incorporation of the geometric phase in general single potential energy surface dynamics: A removable approximation to ab initio data. *Journal of Chemical Physics*, **2016**, 145, 234111	3.9	24
101	Electronic structure aspects of the spin-forbidden reaction CH3(X 2A2″)+N(4S)→HCN(X 1Σ+)+H2(X 1Σg+). *Journal of Chemical Physics*, **1997**, 107, 4994-4999	3.9	23
100	Photodissociation of the vinoxy radical through conical, and avoided, intersections. *Journal of Chemical Physics*, **2002**, 117, 7198-7206	3.9	23
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98	Theoretical studies of spin-forbidden radiationless decay in polyatomic systems. II. Radiationless decay of a-N2O2. *Journal of Chemical Physics*, **1993**, 98, 3845-3849	3.9	23
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95	Spin-orbit coupling and conical intersections 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. *Journal of Chemical Physics*, **2002**, 116, 2825-2835	3.9	22

94	On the quenching of Na(2P) by HCl: Nonadiabatic effects. *Journal of Chemical Physics*, **1987**, 86, 4990-4996	3.9	22
93	Accurate Neural Network Representation of the Ab Initio Determined Spin-Orbit Interaction in the Diabatic Representation Including the Effects of Conical Intersections. *Journal of Physical Chemistry Letters*, **2020**, 11, 1848-1858	6.4	21
92	On the origin of the heavy atom effect in the fine-structure splitting of the 1 2□state of alkali metal 2P-rare gas van der Waals molecules. *Journal of Chemical Physics*, **1997**, 107, 7690-7694	3.9	21
91	Marching along ridges. An extrapolatable approach to locating conical intersections. *Faraday Discussions*, **2004**, 127, 325-36	3.6	21
90	Statistical and nonstatistical nonadiabatic photodissociation from the first excited state of the hydroxymethyl radical. *Journal of Chemical Physics*, **2005**, 122, 84316	3.9	21
89	A theoretical description of the radiative decay processes (b 1□, a 1□→X 3□n NF. *Journal of Chemical Physics*, **1986**, 85, 7261-7267	3.9	21
88	On the characterization of three state conical intersections: a quasianalytic theory using a group homomorphism approach. *Journal of Chemical Physics*, **2006**, 124, 124109	3.9	20
87	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. *Journal of Chemical Physics*, **2001**, 115, 5066-5075	3.9	20
86	On the electronic structure and dynamical aspects of the predissociation of the A 2□states of MgCl. A rigorous quantum mechanical treatment incorporating spin□orbit and derivative coupling effects. *Journal of Chemical Physics*, **1990**, 93, 6403-6418	3.9	20
85	Constructing diabatic representations using adiabatic and approximate diabatic data--Coping with diabolical singularities. *Journal of Chemical Physics*, **2016**, 144, 044104	3.9	20
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83	The photoelectron spectrum of the isopropoxide anion: nonadiabatic effects due to conical intersections and the spin-orbit interaction. *Journal of Chemical Physics*, **2009**, 130, 154312	3.9	19
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75	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□ *Journal of Physical Chemistry B*, **2002**, 106, 8108-8116	3.4	18
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71	On the representation of coupled adiabatic potential energy surfaces using quasi-diabatic Hamiltonians: description of accidental seams of conical intersection. *Molecular Physics*, **2010**, 108, 2611-2619	1.7	16
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68	Predissociation of the c 1□state of NH (ND): The role of dipolar spin□spin coupling. *Journal of Chemical Physics*, **1991**, 94, 2364-2367	3.9	16
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66	On the characterization of three-state conical intersections using a group homomorphism approach: the two-state degeneracy spaces. *Journal of Physical Chemistry B*, **2006**, 110, 19031-9	3.4	15
65	Unanticipated confluences of seams of conical intersection: Reinvestigating intersecting potential-energy surfaces using new tools. I. C(3P)+H2. *Journal of Chemical Physics*, **1998**, 109, 7047-7050	3.9	15
64	On the radiative lifetime of the (a 4□v,N,Fi) levels of the CH radical: An ab initio treatment. *Journal of Chemical Physics*, **1994**, 100, 8991-8998	3.9	15
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62	Insights into the Mechanism of Nonadiabatic Photodissociation from Product Vibrational Distributions. The Remarkable Case of Phenol. *Journal of Physical Chemistry Letters*, **2020**, 11, 191-198	6.4	15
61	Multistate, multichannel coupled diabatic state representations of adiabatic states coupled by conical intersections. CHOH photodissociation. *Journal of Chemical Physics*, **2017**, 146, 134302	3.9	14
60	A Quasi-Diabatic Representation of the 1,2A States of Methylamine. *Journal of Physical Chemistry A*, **2019**, 123, 5231-5241	2.8	14
59	New and Unusual Bonding in Open Shell van der Waals Molecules Revealed by the Heavy Atom Effect: The Case of BAr. *Journal of Physical Chemistry A*, **1997**, 101, 3166-3173	2.8	14

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55	Nonadiabatic Photodissociation of the Hydroxymethyl Radical from the 2(2)A State. Surface Hopping Simulations Based on a Full Nine-Dimensional Representation of the 1,2,3(2)A Potential Energy Surfaces Coupled by Conical Intersections. *Journal of Physical Chemistry A*, **2015**, 119, 7498-509	2.8	13
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49	DETERMINATION OF POTENTIAL ENERGY SURFACE INTERSECTIONS AND DERIVATIVE COUPLINGS IN THE ADIABATIC REPRESENTATION. *Advanced Series in Physical Chemistry*, **2004**, 129-173		12
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