

Millard H Alexander

List of Publications by Year in descending order

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175
papers

7,428
citations

44069

48
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76
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179
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179
docs citations

179
times ranked

1660
citing authors

#	ARTICLE	IF	CITATIONS
1	Rotationally inelastic collisions between a diatomic molecule in a $2^1\Sigma^+$ electronic state and a structureless target. Journal of Chemical Physics, 1982, 76, 5974-5988.	3.0	282
2	Quantum treatment of rotationally inelastic collisions involving molecules in Π electronic states: New derivation of the coupling potential. Chemical Physics, 1985, 92, 337-344.	1.9	256
3	An investigation of the F+H ₂ reaction based on a full ab initio description of the open-shell character of the F(2P) atom. Journal of Chemical Physics, 2000, 113, 11084-11100.	3.0	238
4	Adiabatic and diabatic potential energy surfaces for collisions of CN($X^2\Sigma^+$, $A^2\Pi$) with He. Journal of Chemical Physics, 1988, 89, 3139-3151.	3.0	208
5	Breakdown of the Born-Oppenheimer Approximation in the F+ O_2 -D \rightarrow DF + D Reaction. Science, 2007, 317, 1061-1064.	12.6	149
6	Rotationally inelastic collisions between a diatomic molecule in a $2^1\Sigma^+$ electronic state and a structureless target. Journal of Chemical Physics, 1982, 76, 3637-3645.	3.0	147
7	Theoretical Study of the Validity of the Born-Oppenheimer Approximation in the Cl + H ₂ \rightarrow HCl + H Reaction. Science, 2002, 296, 715-718.	12.6	138
8	Clarification of the electronic asymmetry in Π state doublets with some implications for molecular collisions. Journal of Chemical Physics, 1984, 80, 4325-4332.	3.0	136
9	Spin-orbit effects in the reaction of F(2P) with H ₂ . Journal of Chemical Physics, 1998, 109, 5710-5713.	3.0	131
10	The inelastic scattering of $2^1\Sigma$ [case (b)] molecules and an understanding of the differing Π doublet propensities for molecules of Π vs Σ orbital occupancy. Journal of Chemical Physics, 1989, 91, 839-848.	3.0	130
11	Spin-orbit branching in the photofragmentation of HCl. Journal of Chemical Physics, 1993, 99, 1752-1764.	3.0	114
12	Quantum scattering studies of electronically inelastic collisions of CN ($X^2\Sigma^+$, $A^2\Pi$) with He. Journal of Chemical Physics, 1989, 91, 5425-5439.	3.0	113
13	A new, fully ab initio investigation of the NO($X^2\Pi$)Ar system. I. Potential energy surfaces and inelastic scattering. Journal of Chemical Physics, 1999, 111, 7426-7434.	3.0	109
14	Fully State-Resolved Differential Cross Sections for the Inelastic Scattering of the Open-Shell NO Molecule by Ar. Science, 2001, 294, 832-834.	12.6	108
15	The rate of the F+H ₂ reaction at very low temperatures. Nature Chemistry, 2014, 6, 141-145.	13.6	105
16	Theoretical study of intramultiplet transitions in collisions of atoms in P^3 electronic states with structureless targets: Ca(P^3)+He. Physical Review A, 1983, 28, 73-82.	2.5	103
17	Differential and integral cross sections for the inelastic scattering of NO ($X^2\Pi$) by Ar based on a new ab initio potential energy surface. Journal of Chemical Physics, 1993, 99, 7725-7738.	3.0	99
18	Spectroscopic observation of resonances in the F + H O_2 reaction. Science, 2015, 349, 510-513.	12.6	98

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19	The Extent of Non-Born-Oppenheimer Coupling in the Reaction of Cl(² P) with <i>para</i> -H ₂ . Science, 2008, 322, 573-576.	12.6	95
20	Collision induced transitions between 2^1 and 2^3 states of diatomic molecules: Quantum theory and collisional propensity rules. Journal of Chemical Physics, 1986, 84, 100-113.	3.0	94
21	Propensity rules in rotationally inelastic collisions of diatomic molecules in 3^1 electronic states. Journal of Chemical Physics, 1983, 79, 302-310.	3.0	86
22	Collision-induced transitions between molecular hyperfine levels: Quantum formalism, propensity rules, and experimental study of CaBr(2^1 +)+Ar. Journal of Chemical Physics, 1985, 83, 2191-2200.	3.0	86
23	Quantum interpretation of fully state-selected rotationally inelastic collision experiments. Journal of Chemical Physics, 1977, 66, 59-66.	3.0	82
24	Quantum studies of inelastic collisions of NO(2^1) with Ar. Journal of Chemical Physics, 1983, 79, 6006-6016.	3.0	81
25	Energetics and spin- and λ -doublet selectivity in the infrared multiphoton dissociation HN ₃ ($1A^1$) \rightarrow N ₂ (1^1 +g)+NH(3^1 , 1^1): Theory. Journal of Chemical Physics, 1988, 89, 1388-1400.	3.0	78
26	The infinite-order sudden approximation for collisions involving molecules in 1^1 electronic states: A new derivation and calculations of rotationally inelastic cross sections for NO(2^1)+He and Ar. Journal of Chemical Physics, 1986, 85, 5652-5659.	3.0	77
27	A decoupled λ -dominant approximation for ion-molecule and atom-molecule collisions. Journal of Chemical Physics, 1976, 64, 3009-3013.	3.0	75
28	A combined experimental and theoretical study of rotational energy transfer in collisions between NO($2^1_{1/2}$, $\nu=3, J$) and He, Ar and N ₂ at temperatures down to 7 K. Journal of Chemical Physics, 1998, 109, 3882-3897.	3.0	74
29	Nonadiabatic Interactions in the Cl + H ₂ Reaction Probed by ClH ₂ ⁺ and CID ⁺ Photoelectron Imaging. Science, 2008, 319, 72-75.	12.6	74
30	Adiabatic and approximate diabatic potential energy surfaces for the B...H ₂ van der Waals molecule. Journal of Chemical Physics, 1993, 99, 6014-6026.	3.0	73
31	Rotationally inelastic scattering of two HF molecules. Journal of Chemical Physics, 1977, 66, 1334-1342.	3.0	70
32	Product multiplet branching in the O(1D)+H ₂ \rightarrow OH(2^1)+H reaction. Journal of Chemical Physics, 2004, 121, 5221-5235.	3.0	69
33	An λ -dominant simplification of the close-coupled equations for collisions between atoms and diatomic molecules. Journal of Chemical Physics, 1975, 63, 3552-3559.	3.0	67
34	Theoretical study of Ca(4s5p $1P$) \rightarrow Ca(4s5p $3P$) transitions in collisions with He: Integral cross sections and alignment effects. Journal of Chemical Physics, 1987, 86, 4790-4800.	3.0	67
35	Potential energy surfaces for the interaction of BH(1^1 + 1^1) with Ar and a theoretical investigation of the stretch-bend levels of the ArBH(A) van der Waals molecule. Journal of Chemical Physics, 1994, 101, 2887-2902.	3.0	67
36	Hybrid quantum scattering algorithms for long-range potentials. Journal of Chemical Physics, 1984, 81, 4510-4516.	3.0	65

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37	Semiempirical potential surfaces and dynamical considerations for collisions between alkali metals and molecular oxygen: $\text{Li} + \text{O}_2$ and $\text{Na} + \text{O}_2$. <i>Journal of Chemical Physics</i> , 1978, 69, 3502-3517.	3.0	60
38	Dipolar model for collisional energy transfer between dark and radiating excited electronic states: $\text{CaO}(\text{A}^2\text{I}, \text{a}^3\text{I}) + \text{N}_2\text{O} \rightarrow \text{CaO}(\text{A}^2\text{I}^+) + \text{N}_2\text{O}$. <i>Journal of Chemical Physics</i> , 1982, 76, 429-444.	3.0	59
39	State-to-state inelastic scattering of Stark-decelerated OH radicals with Ar atoms. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 10660.	2.8	57
40	Fitting an ab initio HF \rightarrow HF potential surface. <i>Journal of Chemical Physics</i> , 1976, 65, 5009-5016.	3.0	56
41	Potential surface dependence of vibrationally inelastic collisions between He and H ₂ . <i>Journal of Chemical Physics</i> , 1974, 60, 3950-3957.	3.0	55
42	Potential energy surfaces for the interaction of CH($X^2\text{B}, \text{B}^2\text{A}''$) with Ar and an assignment of the stretch \rightarrow bend levels of the ArCH(B) van der Waals molecule. <i>Journal of Chemical Physics</i> , 1994, 101, 4547-4560.	3.0	55
43	LiH state \rightarrow state rotationally inelastic cross sections in collisions with HCl and DCl. <i>Journal of Chemical Physics</i> , 1979, 71, 1670-1682.	3.0	54
44	Ab initio potential energy surfaces and quantum scattering studies of NO($X^2\text{I}$) with He: $\hat{\nu}$ doublet resolved rotational and electronic fine \rightarrow structure transitions. <i>Journal of Chemical Physics</i> , 1995, 103, 6973-6983.	3.0	53
45	A joint experimental and theoretical study of $\text{A}^2\text{I}^+ \text{X}^2\text{I} +$ electronic energy transfer in the CN molecule induced by collisions with helium. <i>Journal of Chemical Physics</i> , 1993, 98, 8580-8592.	3.0	52
46	On the physical origin of propensity rules in collisions involving molecules in $2^1\Sigma$ electronic states. <i>Journal of Chemical Physics</i> , 1986, 84, 3049-3058.	3.0	51
47	Effective potential study of rotationally \rightarrow vibrationally inelastic collisions between He and H ₂ . <i>Journal of Chemical Physics</i> , 1974, 61, 5167-5181.	3.0	50
48	Quantum close \rightarrow coupled studies of collisions of NO($X^2\text{I}$) with a Ag(111) surface. <i>Journal of Chemical Physics</i> , 1987, 87, 3218-3231.	3.0	49
49	Rotationally inelastic collisions of LiH with He. II. Theoretical treatment of the dynamics. <i>Journal of Chemical Physics</i> , 1980, 72, 6452-6461.	3.0	48
50	Details and consequences of the nonadiabatic coupling in the $\text{Cl}(2\text{P}) + \text{H}_2$ reaction. <i>Faraday Discussions</i> , 2004, 127, 59-72.	3.2	48
51	Quantum flux redistribution during molecular photodissociation. <i>Journal of Chemical Physics</i> , 1992, 97, 2527-2535.	3.0	47
52	Quantum theory of inelastic collisions of a diatomic molecule in a $2^1\Sigma$ electronic state with an uncorrugated surface: $\hat{\nu}$ doublet, spin \rightarrow orbit, and polarization effects in NO ($X^2\text{I}$) \rightarrow Ag (111) scattering. <i>Journal of Chemical Physics</i> , 1984, 80, 3485-3493.	3.0	46
53	Probabilities for classically forbidden transitions using classical and classical path methods. <i>Journal of Chemical Physics</i> , 1976, 65, 2416-2428.	3.0	45
54	Communication: Non-adiabatic coupling and resonances in the F + H ₂ reaction at low energies. <i>Journal of Chemical Physics</i> , 2011, 134, 231101.	3.0	45

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55	Theoretical investigation of weakly-bound complexes of B with H ₂ . Journal of Chemical Physics, 1995, 103, 7956-7965.	3.0	44
56	Low-energy inelastic collisions of OH radicals with He atoms and D^2 molecules. Physical Review A, 2010, 82, .	2.5	44
57	Inelastic collisions of OH($X^2\tilde{1}$) with para-H ₂ : $\tilde{1}$ -doublet and hyperfine-structure transitions. Journal of Chemical Physics, 1988, 88, 6931-6937.	3.0	43
58	Lack of M-preserving propensities in rotationally inelastic collisions of NO($X^2\tilde{1}/2$). Journal of Chemical Physics, 1984, 80, 4133-4136.	3.0	40
59	Polarization and M-dependent effects in rotationally inelastic collisions of open-shell diatomic molecules: Ar-NO($X^2\tilde{1}/2$). Journal of Chemical Physics, 1984, 80, 1506-1516.	3.0	40
60	Tensor cross sections and collisional depolarization of OH($X^2\tilde{1}$) in collisions with helium. Journal of Chemical Physics, 2009, 130, 164315.	3.0	40
61	Scattering of NH ₃ by ortho- and para-H ₂ : Expansion of the potential and collisional propensity rules. Journal of Chemical Physics, 1993, 98, 4662-4671.	3.0	38
62	Time-dependent wavepacket investigation of state-to-state reactive scattering of Cl with <i>i</i> -H ₂ including the open-shell character of the Cl atom. Journal of Chemical Physics, 2010, 132, 034308.	3.0	38
63	On the generation of preferential $\tilde{1}$ -doublet populations in the collisional relaxation of highly rotationally excited CH($X^2\tilde{1}$). Journal of Chemical Physics, 1994, 101, 7468-7479.	3.0	36
64	Experimental and theoretical study of the B-Ne nonbonding interaction: The free-bound $B^2\tilde{1} + X^2\tilde{1}$ electronic transition. Journal of Chemical Physics, 1995, 103, 2779-2786.	3.0	36
65	A new, fully ab initio investigation of the ArNO($X^2\tilde{1}$) system. II. Bound states of the Ar-NO complex. Journal of Chemical Physics, 1999, 111, 7435-7439.	3.0	36
66	Experimental and theoretical study of rotationally inelastic collisions of highly rotationally excited CN($A^2\tilde{2}$) with Ar. Journal of Chemical Physics, 2000, 112, 4474-4484.	3.0	36
67	The dynamics of the prototype abstraction reaction Cl(2P _{3/2} ,1/2)+ H ₂ : A comparison of crossed molecular beam experiments with exact quantum scattering calculations on coupled ab initio potential energy surfaces. Physical Chemistry Chemical Physics, 2004, 6, 5007.	2.8	36
68	Mechanism of and alignment effects in spin-changing collisions involving atoms in 1P electronic states: Ca(4s5p ¹ P)+noble gases. Journal of Chemical Physics, 1989, 90, 5373-5385.	3.0	35
69	Theoretical investigation of weakly-bound complexes of O(3P) with H ₂ . Journal of Chemical Physics, 1998, 108, 4467-4477.	3.0	35
70	dominant study of rotationally inelastic Li+H ₂ collisions. Journal of Chemical Physics, 1975, 63, 5327-5332.	3.0	34
71	Rotational alignment in inelastic collisions. Journal of Chemical Physics, 1977, 66, 4126-4132.	3.0	34
72	Resonances in rotationally inelastic scattering of NH ₃ and ND ₃ with H ₂ . Journal of Chemical Physics, 2015, 143, 044312.	3.0	34

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73	Rotationally inelastic scattering of OH by molecular hydrogen: Theory and experiment. Journal of Chemical Physics, 2015, 142, 204310.	3.0	34
74	Enhanced reactivity of fluorine with para-hydrogen in cold interstellar clouds by resonance-induced quantum tunnelling. Nature Chemistry, 2019, 11, 744-749.	13.6	34
75	Further studies of 4He-H_2 vibrational relaxation. Journal of Chemical Physics, 1977, 66, 4608-4615.	3.0	33
76	A collaborative theoretical and experimental study of the structure and electronic excitation spectrum of the Ba and Ba_2 complexes. Journal of Chemical Physics, 1997, 106, 6320-6331.	3.0	33
77	The study of flux redistribution during molecular photodissociation: Adiabatic and diabatic analyses and application to the dissociation of CH_3I . Journal of Chemical Physics, 1992, 97, 4836-4845.	3.0	31
78	A joint theoretical-experimental investigation of the lower bound states of the $\text{NO}(\text{X}^2\Sigma^+)$ -Ar complex. Journal of Chemical Physics, 2000, 113, 73-85.	3.0	31
79	Potential energy surfaces for and energetics of the weakly-bound Al-H_2 and B-H_2 complexes. Journal of Chemical Physics, 2000, 112, 5722-5730.	3.0	31
80	Sudden theories of rotationally inelastic LiH-HCl and LiH-DCI collisions. Journal of Chemical Physics, 1979, 71, 1683-1691.	3.0	30
81	Propensity rules for rotationally inelastic collisions of symmetric top molecules or linear polyatomic molecules with structureless atoms. Journal of Chemical Physics, 1982, 77, 1855-1865.	3.0	30
82	Theoretical study of $\text{Ca}(4s5p^1P^1)$, $\text{Ca}(4s5p^3P)$ transitions in collision with noble gases: Integral cross sections and alignment effects. Journal of Chemical Physics, 1989, 91, 1658-1667.	3.0	30
83	Quantum study of the redistribution of flux during inelastic collisions. Journal of Chemical Physics, 1991, 95, 8931-8940.	3.0	30
84	Theoretical investigation of the lower bend-stretch states of the Cl^-H_2 anion complex and its isotopomers. Journal of Chemical Physics, 2003, 118, 9637-9642.	3.0	30
85	Experimental and theoretical study of rotationally inelastic polar molecule collisions: 7LiH-HCN . Journal of Chemical Physics, 1980, 72, 6513-6520.	3.0	29
86	A selection rule for M -dependent transitions in collisional excitation of open shell diatomics. Journal of Chemical Physics, 1983, 78, 800-806.	3.0	29
87	Inelastic collisions of $\text{CaCl}(\text{X}^2\Sigma^+)$ with Ar: A collaborative theoretical and experimental study. Journal of Chemical Physics, 1985, 83, 556-566.	3.0	29
88	Close-coupling studies of rotationally inelastic HF-HF collisions at hyperthermal energies. Journal of Chemical Physics, 1980, 73, 5135-5146.	3.0	28
89	Theoretical Study of Bound States of Ar-NO. The Journal of Physical Chemistry, 1994, 98, 1073-1079.	2.9	28
90	The rotational relaxation of $\text{NH}(\text{c}^1\text{I})$ in collisions with Ar: A combined theoretical and experimental investigation. Journal of Chemical Physics, 1995, 102, 4069-4083.	3.0	28

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91	Experimental investigation of weakly bound B(2p,3s)+H ₂ /D ₂ complexes through laser fluorescence excitation spectroscopy. Journal of Chemical Physics, 1995, 103, 7966-7974.	3.0	28
92	State-resolved inelastic collisions of single rotational, fine structure, and \hat{b} doublet levels of NH(A ³ Σ^+) with helium: A combined experimental and theoretical study. Journal of Chemical Physics, 1996, 104, 1325-1337.	3.0	28
93	State-resolved rotationally inelastic collisions of highly rotationally excited CN(A ² Σ^+) with helium: Influence of the interaction potential. Journal of Chemical Physics, 2001, 115, 8393-8402.	3.0	28
94	Ab initio investigation of bound and predissociating states of the NeOH(X) complex. Journal of Chemical Physics, 1995, 103, 3400-3417.	3.0	27
95	Adiabatic and diabatic potential-energy surfaces of the CN(X ² Σ^+ , A ² Σ^+)Ne complex and nonadiabatic predissociation dynamics. Journal of Chemical Physics, 1997, 107, 7148-7162.	3.0	27
96	Theoretical investigation of rotationally inelastic collisions of CH ₂ (\tilde{X}) with helium. Journal of Chemical Physics, 2011, 134, 154307.	3.0	27
97	Experimental and theoretical study of the AlNe complex. Journal of Chemical Physics, 1998, 108, 3522-3530.	3.0	26
98	The interaction of OH(X ² Σ^+) with H ₂ : Ab initio potential energy surfaces and bound states. Journal of Chemical Physics, 2014, 141, 174309.	3.0	26
99	Angular distributions for the F+H ₂ \rightarrow HF+H reaction: The role of the F spin-orbit excited state and comparison with molecular beam experiments. Journal of Chemical Physics, 2004, 121, 5812-5820.	3.0	24
100	Resonances in rotationally inelastic scattering of OH(X ² Σ^+) with helium and neon. Journal of Chemical Physics, 2012, 136, 144308.	3.0	24
101	Theoretical studies of He(1S)+CH(X ² Σ^+). II. Ab initio cross sections for the inelastic scattering and comparison with experiment. Journal of Chemical Physics, 1994, 100, 1338-1349.	3.0	23
102	Theoretical study of the interaction of AlH(X ¹ Σ^+ , A ¹ Σ^+) with Ar: Potential energy surfaces and bend stretch levels of the ArAlH(X,A) van der Waals complex. Journal of Chemical Physics, 1995, 102, 2413-2425.	3.0	23
103	Clarification of the electronic asymmetry of \hat{b} doublets in $3\hat{1}$ electronic states of diatomic molecules. Journal of Chemical Physics, 1987, 87, 7118-7124.	3.0	22
104	A theoretical study of alignment effects in collisions of N ₂ with a Ag surface. Journal of Chemical Physics, 1987, 87, 4937-4947.	3.0	22
105	Joint Experimental/Theoretical Investigation of the Lower Bound States of the NO(X ² Σ^+)-Kr Complex. Journal of Physical Chemistry A, 2009, 113, 7366-7375.	2.5	22
106	Adiabatic representations for the study of flux redistribution during photodissociation involving coupled electronic states: The effect of vibrational excitation on the photofragmentation of CH ₃ I. Journal of Chemical Physics, 1993, 98, 6196-6207.	3.0	21
107	Role of van der Waals resonances in the vibrational relaxation of HF by collisions with H atoms. Journal of Chemical Physics, 2007, 127, 114301.	3.0	21
108	A semiclassical treatment of rotationally electronically inelastic scattering of NO from Ag(111). Journal of Chemical Physics, 1989, 90, 575-586.	3.0	20

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109	Theoretical investigation of rotationally inelastic collisions of the methyl radical with helium. <i>Journal of Chemical Physics</i> , 2011, 135, 064306.	3.0	20
110	Theoretical investigation of rotationally inelastic collisions of CH ₂ (X̃ _f) with helium. <i>Journal of Chemical Physics</i> , 2012, 136, 224306.	3.0	20
111	Rotationally inelastic collisions between a molecule in a 2S+1̃ electronic state and an open-shell target: General quantum analysis and experimental measurement of state-resolved cross sections for CaCl(X̃ ₂ +)+NO(X̃ ₂). <i>Journal of Chemical Physics</i> , 1986, 84, 1547-1553.	3.0	19
112	The failure of rigid shell models for rotationally inelastic LiH+He collisions. <i>Journal of Chemical Physics</i> , 1980, 73, 1233-1237.	3.0	18
113	Quantum flux studies of the mechanism of Ca(4s5p̃ _{1P})+Ca(4s5p̃ _{3P}) collisions. <i>Journal of Chemical Physics</i> , 1992, 96, 6672-6680.	3.0	18
114	Inelastic collisions of fine structure and ̃-doublet resolved rotational states of PH(Ã ₃ ,̃ _{v=0}) with helium. <i>Journal of Chemical Physics</i> , 1997, 106, 7642-7653.	3.0	18
115	State-to-state rate coefficients for transfer from the rotational levels J = 7.5, 20.5, 31.5 and 40.5 in NO(X̃ ₂ ^{1/2} , v = 2) in collisions with He, Ar and N ₂ and for J=7.5, 20.5 and 31.5 in collisions with NO: comparisons between experiment and theory. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 473-479.	2.8	18
116	Photoabsorption Assignments for the C̃ _f 1B ₂ +̃ _f 1A ₁ Vibronic Transitions of SO ₂ , Using New Ab Initio Potential Energy and Transition Dipole Surfaces. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1012-1021.	2.5	18
117	Fully quantum study of vibrational energy transfer between H ₂ and D ₂ . <i>Journal of Chemical Physics</i> , 1974, 60, 4274-4278.	3.0	17
118	Theory of Stark spectroscopy of molecules in ̃ electronic states: Coherence effects and quantum beats. <i>Journal of Chemical Physics</i> , 1986, 85, 134-145.	3.0	17
119	Potential energy hypersurfaces for the interaction of NO with the Ag(111) surface. <i>Journal of Chemical Physics</i> , 1991, 94, 8454-8467.	3.0	17
120	Flux redistribution during the photodissociation of ClNO in the T ₁ state. <i>Journal of Chemical Physics</i> , 1994, 101, 4722-4734.	3.0	17
121	An ab initio investigation of the O(3P)+H ₂ (1̃ _g) van der Waals well. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 4420-4426.	2.8	17
122	New ab initio adiabatic potential energy surfaces and bound state calculations for the singlet ground X̃ _f 1A ₁ and excited C̃ _f 1B ₂ (21Ã ²) states of SO ₂ . <i>Journal of Chemical Physics</i> , 2016, 144, 174301.	3.0	17
123	The interaction of NO(X̃ ₂) with H ₂ : ab initio potential energy surfaces and bound states. <i>Journal of Chemical Physics</i> , 2017, 146, 114301.	3.0	17
124	A log-derivative propagation scheme for the exact solution of two-state curve crossing problems. <i>Journal of Chemical Physics</i> , 1989, 91, 2388-2395.	3.0	16
125	Rotationally inelastic scattering of CD ₃ and CH ₃ with He: comparison of velocity map-imaging data with quantum scattering calculations. <i>Chemical Science</i> , 2013, 4, 4199.	7.4	16
126	Exact quantum scattering calculations of transport properties for the H ₂ O+H system. <i>Journal of Chemical Physics</i> , 2013, 139, 194309.	3.0	16

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127	Validity of energy gap representations of rotationally inelastic cross sections between polar molecules. <i>Journal of Chemical Physics</i> , 1980, 73, 3797-3803.	3.0	15
128	Collisional effects in Stark spectroscopy of molecules in $1^1\Sigma$ electronic states. <i>Journal of Chemical Physics</i> , 1985, 83, 3340-3348.	3.0	15
129	Rotationally inelastic collisions between a diatomic molecule in a $2S+1^1\Sigma$ electronic state and a $2S$ atom: The optimal choice for the total \hat{e}_i representation. <i>Journal of Chemical Physics</i> , 1985, 83, 5060-5067.	3.0	15
130	Collisions of $\text{NO}(X^2\Pi)$ with a $\text{Ag}(111)$ surface: New quantum scattering studies based on a semiempirical potential energy surface. <i>Journal of Chemical Physics</i> , 1991, 94, 8468-8478.	3.0	15
131	Experimental and theoretical investigation of the rotational structure of the $\text{Al}^+\text{H}_2/\text{D}_2$ complex. <i>Journal of Chemical Physics</i> , 2001, 114, 8938-8947.	3.0	15
132	A simple theoretical study of the CH_2^+ photoelectron spectrum. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 4984.	2.8	15
133	State-to-state quantum dynamics of the $\text{F} + \text{HCl} (v_i = 0, j_i = 0) \rightarrow \text{HF}(v_f, j_f) + \text{Cl}$ reaction on the ground state potential energy surface. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 15347.	2.8	15
134	Semiclassical S -matrix theory of vibrationally inelastic collisions between two diatomic molecules. <i>Journal of Chemical Physics</i> , 1974, 61, 3967-3976.	3.0	14
135	Model studies of the kinetics of collisional population transfer between dark and radiating excited electronic states: $\text{CaO}(A^2\Pi) + \text{N}_2\text{O} \rightarrow \text{CaO}(A^2\Pi) + \text{N}_2\text{O}$. <i>Journal of Chemical Physics</i> , 1982, 77, 839-853.	3.0	14
136	Experimental and theoretical study of the electronic spectrum of the BAr_2 complex: Transition to the excited valence $\text{B}(2s2p^2^3D)$ state. <i>Journal of Chemical Physics</i> , 2000, 112, 5037-5043.	3.0	14
137	Exact quantum scattering calculations of transport properties: $\text{CH}_2(X^3\Sigma^-)$. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7843-7853.	3.0	14
138	State-Specific Collision Dynamics of Molecular Super Rotors with Oriented Angular Momentum. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12471-12479.	2.5	14
139	Inelastic collisions of $\text{CaF}(A^2\Pi)$ with He and Ar: Quantum calculations and adiabatic analysis. <i>Journal of Chemical Physics</i> , 1988, 88, 3581-3589.	3.0	13
140	Electronic spectroscopy and excited state dynamics of the $\text{Al}^+\text{H}_2/\text{D}_2$ complex. <i>Faraday Discussions</i> , 2001, 118, 387-404.	3.2	13
141	Depolarization in $\text{H}_2^+\text{O}^+\text{He}$ collisions. <i>Molecular Physics</i> , 2010, 108, 1159-1169.	1.7	13
142	Transport Properties for Systems with Deep Potential Wells: $\text{H} + \text{O}_2$. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11935-11942.	2.5	13
143	Inelastic contributions to ion-molecule diffusion cross sections: Li^+H_2 . <i>Journal of Chemical Physics</i> , 1976, 64, 4498-4503.	3.0	12
144	Experimental and theoretical study of \hat{b} -doublet resolved rotationally inelastic collisions of highly rotationally excited $\text{CH}(A^2\Sigma^+, v=0)$ with Ar. <i>Journal of Chemical Physics</i> , 2001, 115, 800-809.	3.0	12

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145	Experimental and Theoretical Study of State-Resolved Electronically Inelastic Collisions of Highly Rotationally Excited CN(A ₂) with Argon and Helium: The Role of Gateway Levels. <i>Journal of Physical Chemistry A</i> , 2002, 106, 8345-8354.	2.5	12
146	Reactivity of the F spin-orbit excited state in the F + HD reaction: Product translational and rotational energy distributions. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 5018-5025.	2.8	12
147	Experimental and theoretical investigation of the temperature dependent electronic quenching of O(¹ D) atoms in collisions with Kr. <i>Journal of Chemical Physics</i> , 2018, 148, 124311.	3.0	12
148	Exact quantum scattering calculation of transport properties for free radicals: OH(X ²) helium. <i>Journal of Chemical Physics</i> , 2012, 137, 094306.	3.0	11
149	Uncloaking the Quantum Nature of Inelastic Molecular Collisions. <i>Science</i> , 2013, 341, 1076-1077.	12.6	11
150	Accurate transport properties for O(³ P)H and O(³ P)H ₂ . <i>Journal of Chemical Physics</i> , 2016, 145, 164309.	3.0	11
151	On analytic fits to the Gordon-Secrest potential energy surface for HeH ₂ : A reply. <i>Journal of Chemical Physics</i> , 1974, 61, 3868-3869.	3.0	10
152	Nonadiabatic effects in the photodetachment of CH ₂ ⁻ . <i>Journal of Chemical Physics</i> , 2008, 128, 084312.	3.0	10
153	Theoretical study of the vibrational relaxation of the methyl radical in collisions with helium. <i>Journal of Chemical Physics</i> , 2013, 138, 104317.	3.0	10
154	Collision dynamics of symmetric top molecules: A comparison of the rotationally inelastic scattering of CD ₃ and ND ₃ with He. <i>Journal of Chemical Physics</i> , 2014, 140, 134308.	3.0	10
155	Rotational energy transfer in HF: A computational study. <i>Journal of Chemical Physics</i> , 1989, 91, 7563-7589.	3.0	9
156	Laser spectroscopic study of the SiAr van der Waals complex. <i>Journal of Chemical Physics</i> , 2002, 116, 9239-9248.	3.0	9
157	Experimental and theoretical investigation of the AlH $\tilde{3}\Sigma^+$ electronic transition. <i>Journal of Chemical Physics</i> , 2003, 118, 10477-10484.	3.0	9
158	Chemical Kinetics Under Test. <i>Science</i> , 2011, 331, 411-412.	12.6	9
159	Final State Resolved Quantum Predissociation Dynamics of SO ₂ (Clf ¹)B ₂ and Its Isotopomers via a Crossing with a Singlet Repulsive State. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4930-4938.	2.5	9
160	The use of the current density in the analysis of molecular photodissociation. <i>Journal of Chemical Physics</i> , 1994, 101, 8663-8673.	3.0	8
161	Rotationally inelastic collisions between a molecule in a $\tilde{2}\Sigma$ electronic state and a 2S atom: Sudden factorization, scaling, and symmetry relations. <i>Journal of Chemical Physics</i> , 1986, 85, 1859-1865.	3.0	7
162	Theoretical investigation of the dynamics of O(¹ D) $\tilde{3}\Sigma^+$ electronic quenching by collision with Xe. <i>Journal of Chemical Physics</i> , 2015, 143, 054306.	3.0	7

#	ARTICLE	IF	CITATIONS
163	First-principles C band absorption spectra of SO ₂ and its isotopologues. Journal of Chemical Physics, 2017, 146, 154305.	3.0	7
164	Quantum theory and collisional propensity rules for rotationally inelastic collisions between polyatomic molecules (NH ₃ and CO ₂) and an uncorrugated surface. Journal of Chemical Physics, 1988, 89, 790-800.	3.0	5
165	Spin-orbit quenching of Cl(2P _{1/2}) by H ₂ . Journal of Chemical Physics, 2012, 136, 124312.	3.0	4
166	A MATLAB-based finite-element visualization of quantum reactive scattering. I. Collinear atom-diatom reactions. Journal of Chemical Physics, 2014, 141, 024118.	3.0	4
167	Theoretical investigation of intersystem crossing between the \tilde{a}^1A_1 and \tilde{X}^1B_1 states of CH ₂ induced by collisions with helium. Journal of Chemical Physics, 2014, 141, 064312.	3.0	4
168	Electronic quenching of O(1D) by Xe: Oscillations in the product angular distribution and their dependence on collision energy. Journal of Chemical Physics, 2015, 143, 054307.	3.0	4
169	An ab initio based model for the simulation of multiple 2P atoms embedded in a cluster of spherical ligands, with application to Al in solid para-hydrogen. Journal of Chemical Physics, 2002, 117, 5311-5318.	3.0	2
170	Theoretical investigation of the relaxation of the bending mode of $\tilde{m}CH_2(\tilde{X})$ by collisions with helium. Journal of Chemical Physics, 2014, 141, 214305.	3.0	2
171	Chemical Control and Spectral Fingerprints of Electronic Coupling in Carbon Nanostructures. Journal of Physical Chemistry C, 2016, 120, 29476-29483.	3.1	2
172	Accurate characterization of the lowest triplet potential energy surface of SO ₂ with a coupled cluster method. Journal of Chemical Physics, 2019, 150, 144303.	3.0	2
173	A finite-element visualization of quantum reactive scattering. II. Nonadiabaticity on coupled potential energy surfaces. Journal of Chemical Physics, 2015, 142, 034108.	3.0	1
174	Energetics and spin selectivity in the infrared multiphoton dissociation HN ₃ (\tilde{X}^1A_1) + N ₂ ($X^1\Sigma_g^+$) + NH($X^3\Sigma^-_g, a^1\Pi$). AIP Conference Proceedings, 1989, , .	0.4	0
175	Publisher's Note: <i>ab initio</i> adiabatic potential energy surfaces and bound state calculations for the singlet ground \tilde{X}^1A_1 and excited $\tilde{C}^1B_2(2^1A_1)$ states of SO ₂ . [J. Chem. Phys. 144, 174301 (2016)]. Journal of Chemical Physics, 2016, 144, 209901.	0	0