Gerrit C Groenenboom

List of Publications by Year
in descending order

164 papers	5,384 citations	87888 38 h-index	106344 65 g-index
174 all docs	174 docs citations	174 times ranked	3097 citing authors

#	Article	IF	Citations
1	Laser ionisation detection of O(³P_j) atoms in the VUV; application to photodissociation of O₂. Molecular Physics, 2022, 120, .	1.7	3
2	Collisionâ€induced spinâ€orbit relaxation of highly vibrationally excited NO near 1 K. Natural Sciences, 2022, 2, e20210074.	2.1	5
3	Mapping partial wave dynamics in scattering resonances by rotational de-excitation collisions. Nature Chemistry, 2022, 14, 538-544.	13.6	6
4	Ab initio study of the reactivity of ultracold RbSr + RbSr collisions. New Journal of Physics, 2022, 24, 055001.	2.9	3
5	Glory scattering in deeply inelastic molecular collisions. Nature Chemistry, 2022, 14, 664-669.	13.6	11
6	Many-electron dynamics in high-order harmonic generation of niobium: A time-dependent density-functional-theory study. Physical Review A, 2022, 105, .	2.5	1
7	Efficient computational methods for rovibrational transition rates in molecular collisions. Journal of Chemical Physics, 2022, 157, .	3.0	2
8	Quantifying the interplay between fine structure and geometry of an individual molecule on a surface. Physical Review B, 2021, 103, .	3.2	25
9	Molecular Dynamics Simulations of Energy Dissipation on Amorphous Solid Water: Testing the Validity of Equipartition. ACS Earth and Space Chemistry, 2021, 5, 2032-2041.	2.7	7
10	Multi-channel distorted-wave Born approximation for rovibrational transition rates in molecular collisions. Journal of Chemical Physics, 2021, 155, 034105.	3.0	4
11	Paraâ€ortho hydrogen conversion: Solving a 90â€year old mystery. Natural Sciences, 2021, 1, e10002.	2.1	11
12	Lossy quantum defect theory of ultracold molecular collisions. Physical Review A, 2021, 104, .	2.5	13
13	Magnetic anisotropy of individually addressed spin states. Physical Review Research, 2021, 3, .	3.6	2
14	Correlations in rotational energy transfer for NOâ€“D2 inelastic collisions. Journal of Chemical Physics, 2020, 153, 064301.	3.0	5
15	Rotationalâ€“vibrational resonance states. Physical Chemistry Chemical Physics, 2020, 22, 15081-15104.	2.8	10
16	Imaging the onset of the resonance regime in low-energy NO-He collisions. Science, 2020, 368, 626-630.	12.6	68
17	State-to-state scattering of highly vibrationally excited NO at broadly tunable energies. Nature Chemistry, 2020, 12, 528-534.	13.6	20
18	Suppressed and enhanced tunneling ionization of transition-metal atoms and cations: A time-dependent density-functional-theory study on nickel. Physical Review A, 2020, 101, .	2.5	1

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19	Experimental and theoretical investigation of resonances in low-energy NOâ€“H2 collisions. Journal of Chemical Physics, 2020, 153, 244302.	3.0	5
20	Controlling the nature of a charged impurity in a bath of Feshbach dimers. Physical Review Research, 2020, 2, .	3.6	17
21	Quantum spin systems versus Schroedinger operators: A case study in spontaneous symmetry breaking. SciPost Physics, 2020, 8, .	4.9	8
22	Quasiclassical method for calculating the density of states of ultracold collision complexes. Physical Review A, 2019, 100, .	2.5	50
23	Photoinduced Two-Body Loss of Ultracold Molecules. Physical Review Letters, 2019, 123, 123402.	7.8	84
24	Differential Cross Sections for State-to-State Collisions of NO(v = 10) in Near-Copropagating Beams. Journal of Physical Chemistry Letters, 2019, 10, 2422-2427.	4.6	17
25	Update of the HITRAN collision-induced absorption section. Icarus, 2019, 328, 160-175.	2.5	105
26	Six-dimensional potential energy surface for NaKâ€“NaK collisions: Gaussian process representation with correct asymptotic form. Journal of Chemical Physics, 2019, 150, 064106.	3.0	34
27	Diabatic states, nonadiabatic coupling, and the counterpoise procedure for weakly interacting open-shell molecules. Journal of Chemical Physics, 2018, 148, .	3.0	8
28	Correlated energy transfer in rotationally and spinâ€“orbit inelastic collisions of NO(X²Î_{1/2}, j = 1/2f) with O₂(X³Î£_g^{â¯}). Physical Chemistry Chemical Physics, 2018, 20, 12444-12453.	2.8	11
29	O2â¯O2 and O2â¯N2 collision-induced absorption mechanisms unravelled. Nature Chemistry, 2018, 10, 549-554.	13.6	29
30	Scattering resonances in bimolecular collisions between NO radicals and H2 challenge the theoretical gold standard. Nature Chemistry, 2018, 10, 435-440.	13.6	56
31	Observation of correlated excitations in bimolecular collisions. Nature Chemistry, 2018, 10, 469-473.	13.6	32
32	Characterization of methanol as a magnetic field tracer in star-forming regions. Nature Astronomy, 2018, 2, 145-150.	10.1	23
33	Energy dependent parity-pair behavior in NO + He collisions. Journal of Chemical Physics, 2018, 149, 084306.	3.0	2
34	Potential energy and dipole moment surfaces of the triplet states of the O2(X3Î£gâ¯) â¯ O2(X3Î£gâ¯,a1Î”g,b1Î£g+) complex. Journal of Chemical Physics, 2017, 147, 084306.	3.0	14
35	Line-shape theory of the X3Î£gâ¯â†'a1Î”g,b1Î£g+ transitions in O2â€“O2 collision-induced absorption. Journal of Chemical Physics, 2017, 147, 084307.	3.0	9
36	State-to-State Differential Cross Sections for Inelastic Collisions of NO Radicals with para-H₂ and ortho-D₂. Journal of Physical Chemistry A, 2017, 121, 7446-7454.	2.5	13

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37	Tunneling ionization of the F4 and D6 states of vanadium: Exchange blockade. Physical Review A, 2017, 96, .	2.5	2
38	Imaging diffraction oscillations for inelastic collisions of NO radicals with He and D2. Journal of Chemical Physics, 2017, 147, 013918.	3.0	16
39	Imaging quantum stereodynamics through Fraunhofer scattering of NO radicals with rare-gas atoms. Nature Chemistry, 2017, 9, 226-233.	13.6	50
40	Quantum-Chemical calculations revealing the effects of magnetic fields on methanol masers. Proceedings of the International Astronomical Union, 2017, 13, 23-26.	0.0	0
41	Hyperfine interactions and internal rotation in methanol. Journal of Chemical Physics, 2016, 145, 244301.	3.0	16
42	Time-dependent density-functional-theory study of the suppressed tunneling ionization of vanadium. Physical Review A, 2016, 94, .	2.5	4
43	Contributions of inner-valence molecular orbitals and multiphoton resonances to high-order-harmonic generation of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>: A time-dependent	2.5	17
44	Stark Interference of Electric and Magnetic Dipole Transitions in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>A</mml:mi><mml:mo>â^'</mml:mo><mml:mi>X</mml:mi></mml:mrow></mml:math>Band of OH. Physical Review Letters, 2016, 116, 153001.	7.8	2
45	Communication: Multiple-property-based diabatization for open-shell van der Waals molecules. Journal of Chemical Physics, 2016, 144, 121101.	3.0	16
46	Probing Scattering Resonances in (Ultra)Cold Inelastic NOâ€“He Collisions. Journal of Physical Chemistry A, 2016, 120, 4770-4777.	2.5	10
47	QUANTUM CALCULATION OF INELASTIC CO COLLISIONS WITH H. III. RATE COEFFICIENTS FOR RO-VIBRATIONAL TRANSITIONS. Astrophysical Journal, 2015, 813, 96.	4.5	12
48	Collision-induced absorption with exchange effects and anisotropic interactions: Theory and application to H2 â^' H2. Journal of Chemical Physics, 2015, 142, 084305.	3.0	19
49	Imaging resonances in low-energy NO-He inelastic collisions. Science, 2015, 350, 787-790.	12.6	115
50	Resolving rainbows with superimposed diffraction oscillations in NO + rare gas scattering: experiment and theory. New Journal of Physics, 2015, 17, 055019.	2.9	28
51	QUANTUM CALCULATION OF INELASTIC CO COLLISIONS WITH H. II. PURE ROTATIONAL QUENCHING OF HIGH ROTATIONAL LEVELS. Astrophysical Journal, 2015, 811, 27.	4.5	18
52	Quantum mechanical calculation of the collision-induced absorption spectra of N2â€“N2 with anisotropic interactions. Journal of Chemical Physics, 2015, 142, 084306.	3.0	26
53	Quantum scattering calculations for ro-vibrational de-excitation of CO by hydrogen atoms. Journal of Chemical Physics, 2015, 142, 204303.	3.0	11
54	Inelastic Scattering of CO with He: Polarization Dependent Differential State-to-State Cross Sections. Journal of Physical Chemistry A, 2015, 119, 12526-12537.	2.5	14

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55	Direct Extraction of Alignment Moments from Inelastic Scattering Images. Journal of Physical Chemistry A, 2015, 119, 5925-5931.	2.5	10
56	High-Resolution Imaging of Velocity-Controlled Molecular Collisions Using Counterpropagating Beams. Physical Review Letters, 2014, 113, 263202.	7.8	36
57	Cold magnetically trapped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msup><mml:mrow /><mml:mn>2</mml:mn></mml:msup><mml:msub><mml:mi>D</mml:mi><mml:mi>g</mml:mi></mml:msub></mml:mrow></mml:m atoms. I. Interaction potential. Physical Review A, 2014, 90, .	2.5	9
58	Cold magnetically trapped2Dgscandium atoms. II. Scattering dynamics. Physical Review A, 2014, 90, .	2.5	4
59	A theoretical and experimental study of pressure broadening of the oxygen A-band by helium. Journal of Chemical Physics, 2014, 140, 204314.	3.0	8
60	Line strengths of rovibrational and rotational transitions within the ${m X}^3Sigma m {^-}$X3Î£â^' ground state of NH. Journal of Chemical Physics, 2014, 141, 054310.	3.0	31
61	A renormalized potential-following propagation algorithm for solving the coupled-channels equations. Journal of Chemical Physics, 2014, 141, 064102.	3.0	9
62	State-resolved diffraction oscillations imaged for inelastic collisions of NO radicals with He, Ne and Ar. Nature Chemistry, 2014, 6, 216-221.	13.6	101
63	Photodissociation of singlet oxygen in the UV region. Physical Chemistry Chemical Physics, 2014, 16, 3305.	2.8	33
64	Role of resonance-enhanced multiphoton excitation in high-harmonic generation of N2: A time-dependent density-functional-theory study. Physical Review A, 2013, 87, .	2.5	10
65	Quantum Reactive Scattering of Ultracold <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>NH</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mi>X</mml:mi><mml:mtext>â€‰</mml:mtext><mml:mmultiscripts><mml:mi>Î£</mml:mi><mml:mi	7.8	50
66	Three-Dimensional Ab Initio Potential Energy Surface for Hâ€“CO(XÌƒ²Aâ€²). Journal of Physical Chemistry A, 2013, 117, 7571-7579.	2.5	27
67	Communication: Magnetic dipole transitions in the OH Aâ€‰2Î£+ â†•Xâ€‰2Î system. Journal of Chemical Physics, 2012, 137, 101102.	3.0	12
68	Time-dependent density-functional-theory calculation of high-order-harmonic generation of H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review A, 2012, 85, .	2.5	18
69	Scattering resonances in slow NH3â€“He collisions. Journal of Chemical Physics, 2012, 136, 074301.	3.0	51
70	Quantum-State Resolved Bimolecular Collisions of Velocity-Controlled OH with NO Radicals. Science, 2012, 338, 1060-1063.	12.6	114
71	Resonances in rotationally inelastic scattering of OH(X2Î) with helium and neon. Journal of Chemical Physics, 2012, 136, 144308.	3.0	24
72	Towards the complete experiment: measurement of S(1D2) polarization in correlation with single rotational states of CO(J) from the photodissociation of oriented OCS(v2 = 1 | JlM = 111). Physical Chemistry Chemical Physics, 2011, 13, 8549.	2.8	18

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73	Product pair correlation in CH₃OH photodissociation at 157 nm: the OH + CH₃channel. Physical Chemistry Chemical Physics, 2011, 13, 2350-2355.	2.8	21
74	Cold and ultracold NH-NH collisions in magnetic fields. Physical Review A, 2011, 83, .	2.5	38
75	Control and imaging of O(1D2) precession. Nature Chemistry, 2011, 3, 28-33.	13.6	8
76	Scattering of Stark-decelerated OH radicals with rare-gas atoms. European Physical Journal D, 2011, 65, 189-198.	1.3	38
77	On the role of the magnetic dipolar interaction in cold and ultracold collisions: numerical and analytical results for NH(3Î£â¯) + NH(3Î£â¯). European Physical Journal D, 2011, 65, 177-187.	1.3	16
78	Producing translationally cold, ground-state CO molecules. Journal of Chemical Physics, 2011, 135, 114201.	3.0	10
79	Cold and ultracold NHâ€“NH collisions: The field-free case. Journal of Chemical Physics, 2011, 134, 124309.	3.0	20
80	Water dimer vibrationâ€“rotation tunnelling levels from vibrationally averaged monomer wavefunctions. Journal of Quantitative Spectroscopy and Radiative Transfer, 2010, 111, 1262-1276.	2.3	26
81	Angular momentum polarisation in the O(¹D) products of O₂photolysis via the B state. Molecular Physics, 2010, 108, 1145-1157.	1.7	10
82	Photodissociation Imaging of Diatomic Sulfur (S₂). Journal of Physical Chemistry A, 2009, 113, 14995-15005.	2.5	26
83	Photodissociation dynamics of the Aâ€‰Î£2+ state of SH and SD radicals. Journal of Chemical Physics, 2009, 130, 034307.	3.0	21
84	Ab initio potential energy surfaces for NH(Î£3â¯)â€“NH(Î£3â¯) with analytical long range. Journal of Chemical Physics, 2009, 131, 224314.	3.0	42
85	Predissociation of the A2Î£+ (vâ€² = 3) state of the OH radical. Physical Chemistry Chemical Physics, 2009, 11, 4754.	2.8	6
86	Bound states of the OH(Î2)â€“HCl complex on ab initio diabatic potentials. Journal of Chemical Physics, 2009, 131, 124307.	3.0	24
87	Correlated fine structure branching ratios arising from state-selected predissociation of ClO (A2Î3/2). Physical Chemistry Chemical Physics, 2009, 11, 4770.	2.8	8
88	Dynamics of OH(2Î)â€“He collisions in combined electric and magnetic fields. Faraday Discussions, 2009, 142, 127.	3.2	23
89	Cold Collisions of OH(²Î) Molecules with He Atoms in External Fields. Journal of Physical Chemistry A, 2009, 113, 14670-14680.	2.5	20
90	LINEAR RESPONSE TIME DEPENDENT DENSITY FUNCTIONAL THEORY FOR DISPERSION COEFFICIENTS BETWEEN ATOMIC PAIRS. , 2009, , .		0

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91	Photodissociation of vibrationally excited OH/OD radicals. Molecular Physics, 2008, 106, 557-572.	1.7	15
92	New ab initio potential energy surface and the vibration-rotation-tunneling levels of (H2O)2 and (D2O)2. Journal of Chemical Physics, 2008, 128, 034312.	3.0	104
93	Polarizable interaction potential for water from coupled cluster calculations. II. Applications to dimer spectra, virial coefficients, and simulations of liquid water. Journal of Chemical Physics, 2008, 128, 094314.	3.0	85
94	Polarizable interaction potential for water from coupled cluster calculations. I. Analysis of dimer potential energy surface. Journal of Chemical Physics, 2008, 128, 094313.	3.0	91
95	Time-Domain Measurement of Spontaneous Vibrational Decay of Magnetically Trapped NH. Physical Review Letters, 2008, 100, 083003.	7.8	48
96	Photodissociation of vibrationally excited SH and SD radicals at 288 and 291nm: The S(D21) channel. Journal of Chemical Physics, 2007, 126, 094304.	3.0	16
97	Spin-orbit relaxation of Cl(P1âˆ•22) and F(P1âˆ•22) in a gas of H2. Journal of Chemical Physics, 2007, 126, 184303.	3.0	13
98	Electronic anisotropy between open shell atoms in first and second order perturbation theory. Journal of Chemical Physics, 2007, 126, 204306.	3.0	16
99	The radiative lifetime of metastable CO (aÎ3, v=). Journal of Chemical Physics, 2007, 127, 221102.	3.0	93
100	Ab Initio Treatment of the Chemical Reaction Precursor Complex Br(2P)â‹¯HCN. 2. Bound-State Calculations and Infrared Spectraâ€. Journal of Physical Chemistry A, 2007, 111, 7270-7281.	2.5	2
101	Dynamic polarizabilities of rare-earth-metal atoms and dispersion coefficients for their interaction with helium atoms. Physical Review A, 2007, 75, .	2.5	43
102	Theoretical transition probabilities for the OH Meinel system. Journal of Chemical Physics, 2007, 126, 114314.	3.0	126
103	(2+1)REMPI on molecular nitrogen through the 1Î£g+ (II)-state. Chemical Physics Letters, 2007, 435, 242-246.	2.6	13
104	Predictions of the Properties of Water from First Principles. Science, 2007, 315, 1249-1252.	12.6	382
105	Vibrational state-dependent predissociation dynamics of ClO (A2Î3/2): Insight from correlated fine structure branching ratios. Physical Chemistry Chemical Physics, 2006, 8, 2964-2971.	2.8	9
106	Raman association of H2 in the early universe. Faraday Discussions, 2006, 133, 43.	3.2	3
107	Ab Initio Treatment of the Chemical Reaction Precursor Complex Cl(2P)â‹¯HF. 2. Bound States and Infrared Spectrumâ€. Journal of Physical Chemistry A, 2006, 110, 5280-5288.	2.5	12
108	Photolysis of NO2 at multiple wavelengths in the spectral region 200â€“205Ânm. European Physical Journal D, 2006, 38, 151-162.	1.3	23

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109	The photodissociation dynamics of ozone at 193nm: An O(D21) angular momentum polarization study. Journal of Chemical Physics, 2006, 125, 133308.	3.0	22
110	Interaction potential for water dimer from symmetry-adapted perturbation theory based on density functional description of monomers. Journal of Chemical Physics, 2006, 125, 044301.	3.0	61
111	Near-Threshold Inelastic Collisions Using Molecular Beams with a Tunable Velocity. Science, 2006, 313, 1617-1620.	12.6	213
112	Ab initio calculation of the NH(Î£â¯3)â¯NH(Î£â¯3) interaction potentials in the quintet, triplet, and singlet states. Journal of Chemical Physics, 2005, 123, 184302.	3.0	31
113	Ab initiopotential-energy surface for the reaction Ca+HClâ†'CaCl+H. Journal of Chemical Physics, 2005, 122, 204307.	3.0	17
114	Direct Measurement of the Radiative Lifetime of Vibrationally Excited OH Radicals. Physical Review Letters, 2005, 95, 013003.	7.8	93
115	Ab initio computed diabatic potential energy surfaces of OHâ€"HCl. Journal of Chemical Physics, 2005, 122, 244325.	3.0	40
116	Interaction of NH(XÎ£â¯3) with He: Potential energy surface, bound states, and collisional Zeeman relaxation. Journal of Chemical Physics, 2005, 122, 094307.	3.0	74
117	Experimental and theoretical investigation of the A3Îâ€"X3Î£â¯transition of NH/Dâ€"Ne. Physical Chemistry Chemical Physics, 2005, 7, 846-854.	2.8	8
118	Polarizabilities of Sc and Ti atoms and dispersion coefficients for their interaction with helium atoms. Physical Review A, 2005, 72, .	2.5	21
119	Ab initiocalculation of (2+1) resonance enhanced multiphoton ionization spectra and lifetimes of the (D,3)Î£â¯2 states of OH and OD. Journal of Chemical Physics, 2005, 123, 074310.	3.0	15
120	New applications of the genetic algorithm for the interpretation of high-resolution spectra. Canadian Journal of Chemistry, 2004, 82, 804-819.	1.1	81
121	Vibrational predissociation in the HCl dimer. Journal of Chemical Physics, 2004, 120, 9487-9498.	3.0	22
122	Steric asymmetry and lambda-doublet propensities in state-to-state rotationally inelastic scattering of NO(2Î1/2) with He. Journal of Chemical Physics, 2004, 121, 11691-11701.	3.0	34
123	Theoretical study of the Heâ€"HF+ complex. II. Rovibronic states from coupled diabatic potential energy surfaces. Journal of Chemical Physics, 2004, 120, 103-116.	3.0	8
124	Rovibronic spectroscopy of the van der Waals complex Heâ€"HCl+. Molecular Physics, 2004, 102, 2285-2295.	1.7	4
125	Bound States of the Cl(2P)â¯HCl van der Waals Complex from Coupled ab Initio Potential Energy Surfaces. Journal of Physical Chemistry A, 2004, 108, 9319-9322.	2.5	9
126	O(3PJ) Alignment from the Photodissociation of SO2at 193 nmâ€. Journal of Physical Chemistry A, 2004, 108, 7965-7976.	2.5	49

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127	Electronic Interaction Anisotropy between Atoms in Arbitrary Angular Momentum Statesâ€. Journal of Physical Chemistry A, 2004, 108, 8941-8948.	2.5	75
128	Competition between photodetachment and photodissociation in O2â^'. Journal of Chemical Physics, 2003, 119, 8864-8872.	3.0	15
129	Bound States of the Cl(2P)â^'HCl van der Waals Complex from Coupled ab Initio Potential Energy Surfaces. Journal of Physical Chemistry A, 2003, 107, 5110-5121.	2.5	20
130	Spin-flipping transitions in2Î£molecules induced by collisions with structureless atoms. Physical Review A, 2003, 67, .	2.5	65
131	Diabatic intermolecular potentials and bound states of open-shell atomâ€“molecule dimers: Application to the F([sup 2]P)â€“H[sub 2] complex. Journal of Chemical Physics, 2003, 118, 7340.	3.0	22
132	Spectrum and vibrational predissociation of the HF dimer. II. Photodissociation cross sections and product state distributions. Journal of Chemical Physics, 2003, 119, 286-292.	3.0	13
133	Singletâ€“triplet excitation spectrum of the COâ€“He complex. II. Photodissociation and bound-free CO(aâ€Š3Îâ†Xâ€Š1Î£+) transitions. Journal of Chemical Physics, 2003, 119, 141-148.	3.0	9
134	The Heâ€“CaH([sup 2]Î£[sup +]) interaction. II. Collisions at cold and ultracold temperatures. Journal of Chemical Physics, 2003, 118, 7386.	3.0	75
135	Singletâ€“triplet excitation spectrum of the COâ€“He complex. I. Potential surfaces and boundâ€“bound CO(aâ€Š3Îâ†Xâ€Š1Î£+) transitions. Journal of Chemical Physics, 2003, 119, 131-140.	3.0	18
136	Spectrum and vibrational predissociation of the HF dimer. I. Bound and quasibound states. Journal of Chemical Physics, 2003, 119, 277-285.	3.0	28
137	The Heâ€“CaH ([sup 2]Î£[sup +]) interaction. I. Three-dimensional ab initio potential energy surface. Journal of Chemical Physics, 2003, 118, 7380.	3.0	37
138	Photodissociation of the OD radical at 226 and 243 nm. Journal of Chemical Physics, 2003, 119, 9341-9343.	3.0	15
139	Photodissociation of O2 in the Herzberg continuum. I.Ab initiocalculation of potential energy curves and properties. Journal of Chemical Physics, 2002, 116, 1954-1964.	3.0	31
140	Photodissociation of O2 in the Herzberg continuum. II. Calculation of fragment polarization and angular distribution. Journal of Chemical Physics, 2002, 116, 1965-1975.	3.0	37
141	Reassignment of the O2 spectrum just below dissociation threshold based on ab initio calculations. Journal of Chemical Physics, 2002, 117, 5240-5251.	3.0	20
142	Vibrations, Tunneling, and Transition Dipole Moments in the Water Dimer. Journal of Physical Chemistry A, 2001, 105, 6212-6225.	2.5	100
143	Ab initio prediction of the vibration-rotation-tunneling spectrum of HClâ€“(H2O)2. Journal of Chemical Physics, 2001, 115, 3604-3613.	3.0	7
144	Water pair potential of near spectroscopic accuracy. II. Vibrationâ€“rotationâ€“tunneling levels of the water dimer. Journal of Chemical Physics, 2000, 113, 6702-6715.	3.0	109

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145	Three-dimensional ab initio potential energy surface for Heâ€“O2. Journal of Chemical Physics, 2000, 113, 9562-9566.	3.0	52
146	Water Pair and Three-Body Potential of Spectroscopic Quality fromAb InitioCalculations. Physical Review Letters, 2000, 84, 4072-4075.	7.8	102
147	Water pair potential of near spectroscopic accuracy. I. Analysis of potential surface and virial coefficients. Journal of Chemical Physics, 2000, 113, 6687-6701.	3.0	164
148	Discrete variational quantum reactive scattering method with optimal distorted waves. II. Application to the reaction H+O2â†' OH+O. Journal of Chemical Physics, 1998, 108, 5677-5682.	3.0	18
149	Discrete variational quantum reactive scattering method with optimal distorted waves. I. Theory. Journal of Chemical Physics, 1998, 108, 5670-5676.	3.0	3
150	Entrance Channel Effects in the Reaction of Aligned Ca(1P) with HCl. Journal of Physical Chemistry A, 1997, 101, 7558-7566.	2.5	11
151	Heî—¸HF scattering cross sections from an ab initio SAPT potential: confrontation with experiment. Chemical Physics Letters, 1996, 263, 107-112.	2.6	12
152	Semiclassical calculations on the energy dependence of the steric effect for the reaction Ca(1D)+CH3F(jkm=111)â†'CaF+CH3. Journal of Chemical Physics, 1996, 105, 2247-2262.	3.0	7
153	Semiclassical Calculations on the Energy Dependence of the Steric Effect for the Reactions Ca (1D) + CH3X (jkm= 111) â†' CaX + CH3with X = F, Cl, Br. The Journal of Physical Chemistry, 1996, 100, 16072-16081.	2.9	13
154	On the energy dependence of the steric effect for atomâ€“molecule reactive scattering. II. The reaction Ca(1D)+CH3F(JKM=111)â†'CaF(2Î)+CH3. Journal of Chemical Physics, 1994, 101, 7603-7617.	3.0	13
155	On the energy dependence of the steric effect in atomâ€“molecule reactive scattering. I. A quasiclassical approach. Journal of Chemical Physics, 1994, 101, 7592-7602.	3.0	12
156	State-to-state reaction probabilities for Hâˆ' + H2, D2 collisions. Chemical Physics Letters, 1993, 209, 309-314.	2.6	42
157	Combining the discrete variable representation with the Sâ€matrix Kohn method for quantum reactive scattering. Journal of Chemical Physics, 1993, 99, 9681-9696.	3.0	122
158	On the eigenvalues of the s-state radial equation of a spiked harmonic oscillator. Journal of Physics A, 1992, 25, 3427-3433.	1.6	23
159	Size consistent multireference single and double excitation configuration interaction calculations. The multireference coupled electronâ€pair approximation. Journal of Chemical Physics, 1991, 94, 7212-7220.	3.0	55
160	Solving the discretized timeâ€independent SchrÃ¶dinger equation with the Lanczos procedure. Journal of Chemical Physics, 1990, 92, 4374-4379.	3.0	28
161	Semiclassical calculation of the vibrational structure of theBÌƒâ€‰1BuRydberg state oftransâ€diâ€imide fromabinitioconfiguration interaction potential energy surfaces. Journal of Chemical Physics, 1989, 91, 3027-3035.	3.0	2
162	A quantum chemical study on the mechanism of cis-trans isomerization in retinal-like protonated Schiff bases. Journal of the American Chemical Society, 1988, 110, 1406-1415.	13.7	35

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163	Dynamical calculations on the photoisomerization of small polyenes in a nonadiabatic formalism. Journal of Chemical Physics, 1987, 86, 4895-4909.	3.0	35
164	Correlated rotational excitations in NO-CO inelastic collisions. Journal of Chemical Physics, 0, , .	3.0	4