

Ad van der Avoird

List of Publications by Year in descending order

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197
papers

8,297
citations

38660

50
h-index

58464

82
g-index

203
all docs

203
docs citations

203
times ranked

3761
citing authors

#	ARTICLE	IF	CITATIONS
1	Predictions of the Properties of Water from First Principles. <i>Science</i> , 2007, 315, 1249-1252.	6.0	382
2	Density functional calculations of molecular hyperfine interactions in the zero order regular approximation for relativistic effects. <i>Journal of Chemical Physics</i> , 1998, 108, 4783-4796.	1.2	322
3	Density functional calculations of molecular g-tensors in the zero-order regular approximation for relativistic effects. <i>Journal of Chemical Physics</i> , 1997, 107, 2488-2498.	1.2	283
4	N ₂ interaction potential from ab initio calculations, with application to the structure of (N ₂) ₂ . <i>Journal of Chemical Physics</i> , 1980, 72, 6107-6116.	1.2	243
5	From Intermolecular Potentials to the Spectra of van der Waals Molecules, and Vice Versa. <i>Chemical Reviews</i> , 1994, 94, 1931-1974.	23.0	235
6	Quantum dynamics of non-rigid systems comprising two polyatomic fragments. <i>Molecular Physics</i> , 1983, 50, 1025-1043.	0.8	197
7	Water pair potential of near spectroscopic accuracy. I. Analysis of potential surface and virial coefficients. <i>Journal of Chemical Physics</i> , 2000, 113, 6687-6701.	1.2	164
8	Intermolecular Potentials, Internal Motions, and Spectra of van der Waals and Hydrogen-Bonded Complexes. <i>Chemical Reviews</i> , 2000, 100, 4109-4144.	23.0	161
9	An improved intermolecular potential for nitrogen. <i>Journal of Chemical Physics</i> , 1986, 84, 1629-1635.	1.2	142
10	Multipole moments, polarizabilities and anisotropic long range interaction coefficients for N ₂ . <i>Molecular Physics</i> , 1980, 39, 407-425.	0.8	135
11	Anisotropy of long range interactions between linear molecules: H ₂ -H ₂ and H ₂ -He. <i>Molecular Physics</i> , 1979, 37, 159-180.	0.8	121
12	(Heisenberg) exchange and electrostatic interactions between O ₂ molecules: An ab initio study. <i>Journal of Chemical Physics</i> , 1984, 81, 1929-1939.	1.2	117
13	Imaging resonances in low-energy NO-He inelastic collisions. <i>Science</i> , 2015, 350, 787-790.	6.0	115
14	Quantum-State Resolved Bimolecular Collisions of Velocity-Controlled OH with NO Radicals. <i>Science</i> , 2012, 338, 1060-1063.	6.0	114
15	An ab initio intermolecular potential for the carbon monoxide dimer (CO) ₂ . <i>Journal of Chemical Physics</i> , 1990, 92, 7498-7504.	1.2	112
16	A new He-CO interaction energy surface with vibrational coordinate dependence. I. Ab initio potential and infrared spectrum. <i>Journal of Chemical Physics</i> , 1997, 107, 9921-9928.	1.2	109
17	Water pair potential of near spectroscopic accuracy. II. Vibration-rotation tunneling levels of the water dimer. <i>Journal of Chemical Physics</i> , 2000, 113, 6702-6715.	1.2	109
18	Symmetry-adapted perturbation theory of nonadditive three-body interactions in van der Waals molecules. I. General theory. <i>Journal of Chemical Physics</i> , 1995, 103, 8058-8074.	1.2	106

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19	Update of the HITRAN collision-induced absorption section. <i>Icarus</i> , 2019, 328, 160-175.	1.1	105
20	Water Pair and Three-Body Potential of Spectroscopic Quality from Ab Initio Calculations. <i>Physical Review Letters</i> , 2000, 84, 4072-4075.	2.9	102
21	Quantum dynamics of the van der Waals molecule (N ₂) ₂ : An ab initio treatment. <i>Journal of Chemical Physics</i> , 1982, 77, 5664-5681.	1.2	101
22	State-resolved diffraction oscillations imaged for inelastic collisions of NO radicals with He, Ne and Ar. <i>Nature Chemistry</i> , 2014, 6, 216-221.	6.6	101
23	Directly probing anisotropy in atom-molecule collisions through quantum scattering resonances. <i>Nature Physics</i> , 2017, 13, 35-38.	6.5	99
24	Structure, internal mobility, and spectrum of the ammonia dimer: Calculation of the vibration-rotation tunneling states. <i>Journal of Chemical Physics</i> , 1994, 101, 8430-8442.	1.2	97
25	Ab Initio Calculation of the Heisenberg Exchange Interaction between O ₂ Molecules. <i>Physical Review Letters</i> , 1983, 51, 1167-1170.	2.9	93
26	Quantum theoretical calculations of van der Waals interactions between molecules. Anisotropic long range interactions. <i>International Journal of Quantum Chemistry</i> , 1977, 11, 959-970.	1.0	85
27	Ab initio potential energy surface, infrared spectrum, and second virial coefficient of the He-CO complex. <i>Journal of Chemical Physics</i> , 1995, 103, 321-332.	1.2	78
28	Symmetry-adapted perturbation theory calculation of the He-HF intermolecular potential energy surface. <i>Journal of Chemical Physics</i> , 1994, 101, 2811-2824.	1.2	74
29	Tunneling dynamics, symmetry, and far-infrared spectrum of the rotating water trimer. II. Calculations and experiments. <i>Journal of Chemical Physics</i> , 1996, 105, 8051-8063.	1.2	72
30	Vibration-rotation-tunneling states of the benzene dimer: an ab initio study. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 8219.	1.3	72
31	Quantum dynamical resonances in low-energy CO(j=0) He inelastic collisions. <i>Nature Chemistry</i> , 2015, 7, 349-353.	6.6	72
32	van der Waals rovibration levels and the high resolution spectrum of the argon-benzene dimer. <i>Journal of Chemical Physics</i> , 1993, 98, 5327-5336.	1.2	71
33	Ab initio potential energy surface and near-infrared spectrum of the He-C ₂ H ₂ complex. <i>Journal of Chemical Physics</i> , 1995, 102, 8385-8397.	1.2	68
34	Tunneling dynamics, symmetry, and far-infrared spectrum of the rotating water trimer. I. Hamiltonian and qualitative model. <i>Journal of Chemical Physics</i> , 1996, 105, 8034-8050.	1.2	68
35	Imaging the onset of the resonance regime in low-energy NO-He collisions. <i>Science</i> , 2020, 368, 626-630.	6.0	68
36	Rovibrational states of the H ₂ O-H ₂ complex: An ab initio calculation. <i>Journal of Chemical Physics</i> , 2011, 134, 044314.	1.2	67

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37	Intermolecular potential and rovibrational levels of Ar-HF from symmetry-adapted perturbation theory. Journal of Chemical Physics, 1995, 103, 6076-6092.	1.2	66
38	Computational exploration of the six-dimensional vibration-rotation-tunneling dynamics of (NH ₃) ₂ . Journal of Chemical Physics, 1992, 97, 4750-4763.	1.2	64
39	Ab initio collision-induced polarizability, polarized and depolarized Raman spectra, and second dielectric virial coefficient of the helium diatom. Journal of Chemical Physics, 1996, 104, 6997-7007.	1.2	64
40	Ab initio potential-energy surface and rotationally inelastic integral cross sections of the Ar-CH ₄ complex. Journal of Chemical Physics, 1997, 107, 902-913.	1.2	62
41	Predictions for water clusters from a first-principles two- and three-body force field. Journal of Chemical Physics, 2014, 140, 194101.	1.2	61
42	Ab initio valence-bond calculations of the van der Waals interactions between π systems: The ethylene dimer. Journal of Chemical Physics, 1975, 62, 3326-3339.	1.2	59
43	Lattice dynamics of solid N ₂ with an ab initio intermolecular potential. Journal of Chemical Physics, 1980, 73, 5305-5309.	1.2	56
44	Scattering resonances in bimolecular collisions between NO radicals and H ₂ challenge the theoretical gold standard. Nature Chemistry, 2018, 10, 435-440.	6.6	56
45	New CO-CO interaction potential tested by rovibrational calculations. Journal of Chemical Physics, 2005, 122, 054306.	1.2	54
46	Ab initio Studies of long range interactions between ethylene molecules in the multipole expansion. Theoretica Chimica Acta, 1977, 46, 39-62.	0.9	53
47	Unambiguous assignment of the van der Waals modes of benzene-Ar by analysis of the rotationally resolved UV spectra and comparison with multidimensional calculations. Journal of Chemical Physics, 1996, 104, 882-898.	1.2	53
48	Quantitative characterization of the (D ₂ O) ₃ torsional manifold by terahertz laser spectroscopy and theoretical analysis. Journal of Chemical Physics, 1999, 110, 4369-4381.	1.2	53
49	DYNAMICS OF CO IN AMORPHOUS WATER-ICE ENVIRONMENTS. Astrophysical Journal, 2014, 781, 16.	1.6	52
50	Scattering resonances in slow NH ₃ -He collisions. Journal of Chemical Physics, 2012, 136, 074301.	1.2	51
51	Quantum Reactive Scattering of Ultracold NH_3 X^{\dagger}	2.9	50
52	Imaging quantum stereodynamics through Fraunhofer scattering of NO radicals with rare-gas atoms. Nature Chemistry, 2017, 9, 226-233.	6.6	50
53	Ab initio potential energy surfaces of Ar-NH ₃ for different NH ₃ umbrella angles. Journal of Chemical Physics, 1991, 94, 491-500.	1.2	49
54	Quantitative characterization of the water trimer torsional manifold by terahertz laser spectroscopy and theoretical analysis. II. (H ₂ O) ₃ . Journal of Chemical Physics, 1999, 111, 7789-7800.	1.2	49

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55	Ab Initio Potential Energy Surface and Infrared Spectrum of the Ne ⁺ CO Complex. Journal of Physical Chemistry A, 1997, 101, 4690-4698.	1.1	48
56	Ab initio description of large amplitude motions in solid N ₂ . II. Librons in the \hat{I}^2 phase and the \hat{I}^{\pm} phase transition. Journal of Chemical Physics, 1984, 81, 3658-3665.	1.2	47
57	Magnetic coupling and dynamics in solid \hat{I}^{\pm} and \hat{I}^2 O ₂ . I. An ab initio theoretical approach. Journal of Chemical Physics, 1987, 86, 3583-3596.	1.2	45
58	Infrared spectra of the van der Waals molecule (N ₂) ₂ . Molecular Physics, 1985, 55, 11-32.	0.8	42
59	Ab initio potential energy surfaces of Ar ⁺ H ₂ O and Ar ⁺ D ₂ O. Journal of Chemical Physics, 1991, 94, 8096-8104.	1.2	41
60	Infrared spectroscopy and ab initio potential energy surface for Ne ⁺ C ₂ H ₂ and Ne ⁺ C ₂ HD complexes. Journal of Chemical Physics, 1998, 109, 8968-8979.	1.2	41
61	Quantum calculation of vibrational states in the aniline ⁺ argon van der Waals cluster. Journal of Chemical Physics, 1993, 98, 2709-2719.	1.2	40
62	Terahertz vibration ⁺ rotation ⁺ tunneling spectroscopy of water clusters in the translational band region of liquid water. Journal of Chemical Physics, 2001, 114, 3994-4004.	1.2	40
63	Ab initio computed diabatic potential energy surfaces of OH ⁺ HCl. Journal of Chemical Physics, 2005, 122, 244325.	1.2	40
64	Hartree ⁺ Fock ⁺ Slater ⁺ LCAO calculations on the Cu(II) bis(dithiocarbamate) complex; magnetic coupling parameters and optical spectrum. Journal of Chemical Physics, 1980, 73, 1306-1312.	1.2	39
65	Ab initio description of large amplitude motions in solid N ₂ . I. Librons in the ordered \hat{I}^{\pm} and \hat{I}^3 phases. Journal of Chemical Physics, 1984, 81, 3648-3657.	1.2	39
66	The O ₂ ⁺ O ₂ dimer: Magnetic coupling and spectrum. Journal of Chemical Physics, 1987, 87, 5346-5360.	1.2	39
67	Lattice dynamics of the ethylene crystal with interaction potentials from ab initio calculations. Journal of Chemical Physics, 1978, 69, 5288-5300.	1.2	38
68	The nature of monomer inversion in the ammonia dimer. Journal of Chemical Physics, 1994, 101, 8443-8454.	1.2	38
69	An ab initio CO dimer interaction potential and the computation of the rovibrational spectrum of (CO) ₂ . Physical Chemistry Chemical Physics, 2003, 5, 4767.	1.3	38
70	Cold and ultracold NH-NH collisions in magnetic fields. Physical Review A, 2011, 83, .	1.0	38
71	Vibration and rotation of CO in C ₆₀ and predicted infrared spectrum. Journal of Chemical Physics, 1996, 104, 832-847.	1.2	37
72	Determining the nature of quantum resonances by probing elastic and reactive scattering in cold collisions. Nature Chemistry, 2021, 13, 94-98.	6.6	37

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73	High-Resolution Imaging of Velocity-Controlled Molecular Collisions Using Counterpropagating Beams. <i>Physical Review Letters</i> , 2014, 113, 263202.	2.9	36
74	Higher Energy States in the CO Dimer: Millimeter-Wave Spectra and Rovibrational Calculations. <i>Journal of Physical Chemistry A</i> , 2007, 111, 12238-12247.	1.1	35
75	Ab initio description of large amplitude motions in solid N ₂ . III. Libron-phonon coupling. <i>Journal of Chemical Physics</i> , 1984, 81, 4118-4126.	1.2	34
76	Resonances in rotationally inelastic scattering of NH ₃ and ND ₃ with H ₂ . <i>Journal of Chemical Physics</i> , 2015, 143, 044312.	1.2	34
77	Rotationally inelastic scattering of OH by molecular hydrogen: Theory and experiment. <i>Journal of Chemical Physics</i> , 2015, 142, 204310.	1.2	34
78	The van der Waals rovibrational states of the Ar-NH ₃ dimer. <i>Journal of Chemical Physics</i> , 1991, 94, 501-510.	1.2	33
79	Transformation Properties of Antisymmetric Spin Eigenfunctions under Linear Mixing of the Orbitals. <i>Journal of Chemical Physics</i> , 1972, 57, 2498-2505.	1.2	32
80	Observation of correlated excitations in bimolecular collisions. <i>Nature Chemistry</i> , 2018, 10, 469-473.	6.6	32
81	Vibrational overtones in the electronic ground state of the benzene-Ar complex: A combined experimental and theoretical analysis. <i>Journal of Chemical Physics</i> , 1998, 108, 8408-8417.	1.2	31
82	Near-infrared spectrum and rotational predissociation dynamics of the He-HF complex from an ab initio symmetry-adapted perturbation theory potential. <i>Journal of Chemical Physics</i> , 1994, 101, 2825-2835.	1.2	30
83	Near dissociation states for H ₂ ⁺ He on MRCI and FCI potential energy surfaces. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 24976-24983.	1.3	30
84	Symmetry-adapted perturbation theory of nonadditive three-body interactions in van der Waals molecules. II. Application to the Ar ₂ -HF interaction. <i>Journal of Chemical Physics</i> , 1998, 108, 579-589.	1.2	29
85	Water trimer torsional spectrum from accurate <i>ab initio</i> and semiempirical potentials. <i>Journal of Chemical Physics</i> , 2008, 128, 014302.	1.2	29
86	O ₂ ⁺ O ₂ and O ₂ ⁺ N ₂ collision-induced absorption mechanisms unravelled. <i>Nature Chemistry</i> , 2018, 10, 549-554.	6.6	29
87	Spectrum and vibrational predissociation of the HF dimer. I. Bound and quasibound states. <i>Journal of Chemical Physics</i> , 2003, 119, 277-285.	1.2	28
88	Resolving rainbows with superimposed diffraction oscillations in NO + rare gas scattering: experiment and theory. <i>New Journal of Physics</i> , 2015, 17, 055019.	1.2	28
89	The infrared photodissociation spectra and the internal mobility of SF ₆ , SiF ₄ , and SiH ₄ dimers. <i>Journal of Chemical Physics</i> , 1990, 92, 2837-2847.	1.2	27
90	Overtone vibrational spectroscopy in H ₂ -H ₂ O complexes: A combined high level theoretical <i>ab initio</i> , dynamical and experimental study. <i>Journal of Chemical Physics</i> , 2012, 137, 084301.	1.2	27

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91	Three-Dimensional Ab Initio Potential Energy Surface for H^+CO^+ . Journal of Physical Chemistry A, 2013, 117, 7571-7579.	1.1	27
92	The interaction of $\text{OH}(X^2\text{I})$ with H_2 : Ab initio potential energy surfaces and bound states. Journal of Chemical Physics, 2014, 141, 174309.	1.2	26
93	Quantum mechanical calculation of the collision-induced absorption spectra of N_2^+N_2 with anisotropic interactions. Journal of Chemical Physics, 2015, 142, 084306.	1.2	26
94	Fine structure spectrum of O_2^+ rare gas van der Waals molecules. Journal of Chemical Physics, 1983, 79, 1170-1175.	1.2	25
95	Lattice dynamics of H^+CO from an ab initio potential. Journal of Chemical Physics, 1991, 94, 8402-8407.	1.2	25
96	Potential energy surface and bound states of the NH_3^+Ar and ND_3^+Ar complexes. Journal of Chemical Physics, 2014, 141, 224303.	1.2	25
97	Quantifying the interplay between fine structure and geometry of an individual molecule on a surface. Physical Review B, 2021, 103, .	1.1	25
98	Ab initio Studies of long range interactions between ethylene molecules in the multipole expansion. Theoretica Chimica Acta, 1977, 46, 39-62.	0.9	24
99	Pseudorotation tunneling in several water trimer isotopomers. Journal of Chemical Physics, 1999, 110, 823-831.	1.2	24
100	Bound states of the $\text{OH}(^2\Sigma^+)$ - HCl complex on ab initio diabatic potentials. Journal of Chemical Physics, 2009, 131, 124307.	1.2	24
101	Resonances in rotationally inelastic scattering of $\text{OH}(X^2\text{I})$ with helium and neon. Journal of Chemical Physics, 2012, 136, 144308.	1.2	24
102	Scattering of NH_3 and ND_3 with rare gas atoms at low collision energy. Journal of Chemical Physics, 2015, 143, 184303.	1.2	24
103	Interaction of H_2O with CO : potential energy surface, bound states and scattering calculations. Physical Chemistry Chemical Physics, 2018, 20, 5469-5477.	1.3	24
104	Characterization of methanol as a magnetic field tracer in star-forming regions. Nature Astronomy, 2018, 2, 145-150.	4.2	23
105	The NH_3 umbrella motion in the $\text{Ar}^+\text{-NH}_3$ dimer. Chemical Physics, 1992, 165, 47-55.	0.9	22
106	Diabatic intermolecular potentials and bound states of open-shell atom-molecule dimers: Application to the $\text{F}([^2\Pi])\text{-H}_2$ complex. Journal of Chemical Physics, 2003, 118, 7340.	1.2	22
107	Cold Collisions in a Molecular Synchrotron. Physical Review Letters, 2018, 120, 033402.	2.9	22
108	Stark effect and dipole moments of the ammonia dimer in different vibration-rotation-tunneling states. Journal of Chemical Physics, 1996, 104, 3898-3906.	1.2	20

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109	State-to-state scattering of highly vibrationally excited NO at broadly tunable energies. <i>Nature Chemistry</i> , 2020, 12, 528-534.	6.6	20
110	Differential cross sections for rotational excitation of NH ₃ by collisions with Ar and He: Close coupling results and comparison with experiment. <i>Journal of Chemical Physics</i> , 1996, 105, 3079-3088.	1.2	19
111	The 583.2 GHz torsional hot-band of (D ₂ O) ₃ . <i>Journal of Chemical Physics</i> , 2001, 114, 3988-3993.	1.2	19
112	Collision-induced absorption with exchange effects and anisotropic interactions: Theory and application to H ₂ + H ₂ . <i>Journal of Chemical Physics</i> , 2015, 142, 084305.	1.2	19
113	Singlet-triplet excitation spectrum of the CO-He complex. I. Potential surfaces and bound-bound CO($\tilde{X}^1\Sigma^+$) transitions. <i>Journal of Chemical Physics</i> , 2003, 119, 131-140.	1.2	18
114	Rotationally inelastic scattering of ND ₃ with H ₂ as a probe of the intermolecular potential energy surface. <i>Molecular Physics</i> , 2015, 113, 3925-3933.	0.8	18
115	QUANTUM CALCULATION OF INELASTIC CO COLLISIONS WITH H. II. PURE ROTATIONAL QUENCHING OF HIGH ROTATIONAL LEVELS. <i>Astrophysical Journal</i> , 2015, 811, 27.	1.6	18
116	High-resolution spectroscopy of 4-fluorostyrene-rare gas van der Waals complexes: Results and comparison with theoretical calculations. <i>Journal of Chemical Physics</i> , 1998, 108, 1836-1850.	1.2	17
117	Rotational Spectroscopy of the NH ₃ -H ₂ Molecular Complex. <i>Astrophysical Journal</i> , 2017, 838, 27.	1.6	17
118	Differential Cross Sections for State-to-State Collisions of NO($v=10$) in Near-Copropagating Beams. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 2422-2427.	2.1	17
119	Magnetic coupling and dynamics in solid \hat{I}_\pm and \hat{I}^2 -O ₂ . II. Prediction of magnetic field effects. <i>Journal of Chemical Physics</i> , 1987, 86, 3597-3601.	1.2	16
120	Is the NH ₃ -NH ₃ riddle solved?. <i>Faraday Discussions</i> , 1994, 97, 43-55.	1.6	16
121	Method for the ab initio calculation of intermolecular potentials of ionic clusters: Test on Rg-CO ⁺ , Rg=He, Ne, Ar. <i>Journal of Chemical Physics</i> , 2003, 118, 1110-1118.	1.2	16
122	Hyperfine interactions and internal rotation in methanol. <i>Journal of Chemical Physics</i> , 2016, 145, 244301.	1.2	16
123	Communication: Multiple-property-based diabaticization for open-shell van der Waals molecules. <i>Journal of Chemical Physics</i> , 2016, 144, 121101.	1.2	16
124	Imaging diffraction oscillations for inelastic collisions of NO radicals with He and D ₂ . <i>Journal of Chemical Physics</i> , 2017, 147, 013918.	1.2	16
125	Intramonomer correlation contributions to first-order exchange nonadditivity in trimers. <i>Journal of Chemical Physics</i> , 2000, 112, 3159-3169.	1.2	14
126	Rotational study of the NH ₃ -CO complex: Millimeter-wave measurements and ab initio calculations. <i>Journal of Chemical Physics</i> , 2015, 142, 114308.	1.2	14

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127	Inelastic Scattering of CO with He: Polarization Dependent Differential State-to-State Cross Sections. <i>Journal of Physical Chemistry A</i> , 2015, 119, 12526-12537.	1.1	14
128	Potential energy and dipole moment surfaces of the triplet states of the O ₂ (X ³ Σ ^{-g}) - O ₂ (X ³ Σ ^{-g} , a ¹ Π ^g , b ¹ Σ ^{g+}) complex. <i>Journal of Chemical Physics</i> , 2017, 147, 084306.	1.2	14
129	Direct observation of product-pair correlations in rotationally inelastic collisions of ND ₃ with D ₂ . <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14033-14041.	1.3	14
130	The water-carbon monoxide dimer: new infrared spectra, <i>ab initio</i> rovibrational energy level calculations, and an interesting in-termolecular mode. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14911-14922.	1.3	14
131	Transformation properties of many-electron wave functions with special attention to the relation between pair-correlated DODS and configuration interaction. <i>International Journal of Quantum Chemistry</i> , 1974, 8, 715-732.	1.0	13
132	On the energy dependence of the steric effect for atom-molecule reactive scattering. II. The reaction Ca(1D)+CH ₃ F(jkm=111) → CaF(2 ¹) + CH ₃ . <i>Journal of Chemical Physics</i> , 1994, 101, 7603-7617.	1.2	13
133	Semiclassical Calculations on the Energy Dependence of the Steric Effect for the Reactions Ca(1D) + CH ₃ X(jkm=111) → CaX + CH ₃ with X = F, Cl, Br. <i>The Journal of Physical Chemistry</i> , 1996, 100, 16072-16081.	2.9	13
134	Photodissociation of the methane-argon complex. I. <i>Ab initio</i> intermolecular potential depending on the methane vibrational coordinates. <i>Journal of Chemical Physics</i> , 2002, 117, 7551-7561.	1.2	13
135	Spectrum and vibrational predissociation of the HF dimer. II. Photodissociation cross sections and product state distributions. <i>Journal of Chemical Physics</i> , 2003, 119, 286-292.	1.2	13
136	<i>Ab initio</i> potential-energy surface and rovibrational states of the HCN-HCl complex. <i>Journal of Chemical Physics</i> , 2006, 124, 204315.	1.2	13
137	State-to-State Differential Cross Sections for Inelastic Collisions of NO Radicals with <i>para</i> -H ₂ and <i>ortho</i> -D ₂ . <i>Journal of Physical Chemistry A</i> , 2017, 121, 7446-7454.	1.1	13
138	<i>Ab initio</i> potential and rotational spectra of the CO-N ₂ complex. <i>Journal of Chemical Physics</i> , 2018, 148, 044313.	1.2	13
139	Molecular square dancing in CO-CO collisions. <i>Science</i> , 2020, 369, 307-309.	6.0	13
140	Potential energy surface and bound states of the H ₂ O-HF complex. <i>Journal of Chemical Physics</i> , 2020, 153, 214301.	1.2	13
141	Dynamical and optical properties of the ethylene crystal: Self-consistent phonon calculations using an <i>ab initio</i> intermolecular potential. <i>Journal of Chemical Physics</i> , 1981, 75, 1451-1458.	1.2	12
142	Vibron band structure in chlorinated benzene crystals: Lattice dynamics calculations and Raman spectra of 1,2,4,5-tetrachlorobenzene. <i>Journal of Chemical Physics</i> , 1988, 89, 4023-4034.	1.2	12
143	QUANTUM CALCULATION OF INELASTIC CO COLLISIONS WITH H. III. RATE COEFFICIENTS FOR RO-VIBRATIONAL TRANSITIONS. <i>Astrophysical Journal</i> , 2015, 813, 96.	1.6	12
144	Simulating rotationally inelastic collisions using a direct simulation Monte Carlo method. <i>Molecular Physics</i> , 2015, 113, 3972-3978.	0.8	12

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145	Entrance Channel Effects in the Reaction of Aligned Ca(1P) with HCl. Journal of Physical Chemistry A, 1997, 101, 7558-7566.	1.1	11
146	Quantum scattering calculations for ro-vibrational de-excitation of CO by hydrogen atoms. Journal of Chemical Physics, 2015, 142, 204303.	1.2	11
147	Correlated energy transfer in rotationally and spin-orbit inelastic collisions of NO($X^{2\Sigma^+}$, $v=1/2$) with $O^{2\Sigma^+}$ ($X^{3\Sigma^+}$, $v=0$). Physical Chemistry Chemical Physics, 2018, 20, 12444-12453.	1.3	11
148	Para-ortho hydrogen conversion: Solving a 90-year old mystery. Natural Sciences, 2021, 1, e10002.	1.0	11
149	Rotational study of the CH ₄ -CO complex: Millimeter-wave measurements and ab initio calculations. Journal of Chemical Physics, 2015, 143, 154303.	1.2	11
150	Glory scattering in deeply inelastic molecular collisions. Nature Chemistry, 2022, 14, 664-669.	6.6	11
151	Rotationally Inelastic Scattering of Quantum-State-Selected ND ₃ with Ar. Journal of Physical Chemistry A, 2015, 119, 5979-5987.	1.1	10
152	Direct Extraction of Alignment Moments from Inelastic Scattering Images. Journal of Physical Chemistry A, 2015, 119, 5925-5931.	1.1	10
153	Probing Scattering Resonances in (Ultra)Cold Inelastic NO-He Collisions. Journal of Physical Chemistry A, 2016, 120, 4770-4777.	1.1	10
154	Using a direct simulation Monte Carlo approach to model collisions in a buffer gas cell. Journal of Chemical Physics, 2017, 146, 044302.	1.2	10
155	Rotational-vibrational resonance states. Physical Chemistry Chemical Physics, 2020, 22, 15081-15104.	1.3	10
156	Singlet-triplet excitation spectrum of the CO-He complex. II. Photodissociation and bound-free CO(S_1^+) transitions. Journal of Chemical Physics, 2003, 119, 141-148.	1.2	9
157	The elusive S ₂ state, the S ₁ /S ₂ splitting, and the excimer states of the benzene dimer. Journal of Chemical Physics, 2015, 142, 234306.	1.2	9
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