Ad van der Avoird

List of Publications by Year
in descending order

197	8,297	38742 50	58581 82
papers	citations	h-index	g-index

203	203	203	3761
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Predictions of the Properties of Water from First Principles. Science, 2007, 315, 1249-1252.	12.6	382
2	Density functional calculations of molecular hyperfine interactions in the zero order regular approximation for relativistic effects. Journal of Chemical Physics, 1998, 108, 4783-4796.	3.0	322
3	Density functional calculations of molecular g-tensors in the zero-order regular approximation for relativistic effects. Journal of Chemical Physics, 1997, 107, 2488-2498.	3.0	283
4	N2â€“N2 interaction potential from ab initio calculations, with application to the structure of (N2)2. Journal of Chemical Physics, 1980, 72, 6107-6116.	3.0	243
5	From Intermolecular Potentials to the Spectra of van der Waals Molecules, and Vice Versa. Chemical Reviews, 1994, 94, 1931-1974.	47.7	235
6	Quantum dynamics of non-rigid systems comprising two polyatomic fragments. Molecular Physics, 1983, 50, 1025-1043.	1.7	197
7	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
8	Intermolecular Potentials, Internal Motions, and Spectra of van der Waals and Hydrogen-Bonded Complexes. Chemical Reviews, 2000, 100, 4109-4144.	47.7	161
9	An improved intermolecular potential for nitrogen. Journal of Chemical Physics, 1986, 84, 1629-1635.	3.0	142
10	Multipole moments, polarizabilities and anisotropic long range interaction coefficients for N2. Molecular Physics, 1980, 39, 407-425.	1.7	135
11	Anisotropy of long range interactions between linear molecules: H2-H2 and H2-He. Molecular Physics, 1979, 37, 159-180.	1.7	121
12	(Heisenberg) exchange and electrostatic interactions between O2molecules: Anabinitiostudy. Journal of Chemical Physics, 1984, 81, 1929-1939.	3.0	117
13	Imaging resonances in low-energy NO-He inelastic collisions. Science, 2015, 350, 787-790.	12.6	115
14	Quantum-State Resolved Bimolecular Collisions of Velocity-Controlled OH with NO Radicals. Science, 2012, 338, 1060-1063.	12.6	114
15	An ab initio intermolecular potential for the carbon monoxide dimer (CO)2. Journal of Chemical Physics, 1990, 92, 7498-7504.	3.0	112
16	A new Heâ€“CO interaction energy surface with vibrational coordinate dependence. I. Ab initio potential and infrared spectrum. Journal of Chemical Physics, 1997, 107, 9921-9928.	3.0	109
17	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
18	Symmetryâ€adapted perturbation theory of nonadditive threeâ€body interactions in van der Waals molecules. I. General theory. Journal of Chemical Physics, 1995, 103, 8058-8074.	3.0	106

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19	Update of the HITRAN collision-induced absorption section. Icarus, 2019, 328, 160-175.	2.5	105
20	Water Pair and Three-Body Potential of Spectroscopic Quality fromAb InitioCalculations. Physical Review Letters, 2000, 84, 4072-4075.	7.8	102
21	Quantum dynamics of the van der Waals molecule (N2)2: Anab initiotreatment. Journal of Chemical Physics, 1982, 77, 5664-5681.	3.0	101
22	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
23	Directly probing anisotropy in atomâ€“molecule collisions through quantum scattering resonances. Nature Physics, 2017, 13, 35-38.	16.7	99
24	Structure, internal mobility, and spectrum of the ammonia dimer: Calculation of the vibrationâ€“rotationâ€tunneling states. Journal of Chemical Physics, 1994, 101, 8430-8442.	3.0	97
25	Ab InitioCalculation of the Heisenberg Exchange Interaction betweenO2Molecules. Physical Review Letters, 1983, 51, 1167-1170.	7.8	93
26	Quantum theoretical calculations of van der Waals interactions between molecules. Anisotropic long range interactions. International Journal of Quantum Chemistry, 1977, 11, 959-970.	2.0	85
27	Ab initio potential energy surface, infrared spectrum, and second virial coefficient of the Heâ€“CO complex. Journal of Chemical Physics, 1995, 103, 321-332.	3.0	78
28	Symmetryâ€adapted perturbation theory calculation of the Heâ€“HF intermolecular potential energy surface. Journal of Chemical Physics, 1994, 101, 2811-2824.	3.0	74
29	Tunneling dynamics, symmetry, and farâ€infrared spectrum of the rotating water trimer. II. Calculations and experiments. Journal of Chemical Physics, 1996, 105, 8051-8063.	3.0	72
30	Vibrationâ€“rotation-tunneling states of the benzene dimer: an ab initio study. Physical Chemistry Chemical Physics, 2010, 12, 8219.	2.8	72
31	Quantum dynamical resonances in low-energy CO(jâ€‰=â€‰0)â€‰+â€‰He inelastic collisions. Nature Chemistry, 2015, 7, 349-353.	13.6	72
32	van der Waals rovibration levels and the high resolution spectrum of the argonâ€“benzene dimer. Journal of Chemical Physics, 1993, 98, 5327-5336.	3.0	71
33	Ab initio potential energy surface and nearâ€infrared spectrum of the Heâ€“C2H2 complex. Journal of Chemical Physics, 1995, 102, 8385-8397.	3.0	68
34	Tunneling dynamics, symmetry, and farâ€infrared spectrum of the rotating water trimer. I. Hamiltonian and qualitative model. Journal of Chemical Physics, 1996, 105, 8034-8050.	3.0	68
35	Imaging the onset of the resonance regime in low-energy NO-He collisions. Science, 2020, 368, 626-630.	12.6	68
36	Rovibrational states of the H2Oâ€“H2 complex: An ab initio calculation. Journal of Chemical Physics, 2011, 134, 044314.	3.0	67

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37	Intermolecular potential and rovibrational levels of Arâ€“HF from symmetryâ€adapted perturbation theory. Journal of Chemical Physics, 1995, 103, 6076-6092.	3.0	66
38	Computational exploration of the sixâ€dimensional vibrationâ€“rotationâ€“tunneling dynamics of (NH3)2. Journal of Chemical Physics, 1992, 97, 4750-4763.	3.0	64
39	Ab initiocollisionâ€induced polarizability, polarized and depolarized Raman spectra, and second dielectric virial coefficient of the helium diatom. Journal of Chemical Physics, 1996, 104, 6997-7007.	3.0	64
40	Ab initio potential-energy surface and rotationally inelastic integral cross sections of the Arâ€“CH4 complex. Journal of Chemical Physics, 1997, 107, 902-913.	3.0	62
41	Predictions for water clusters from a first-principles two- and three-body force field. Journal of Chemical Physics, 2014, 140, 194101.	3.0	61
42	Abinitiovalenceâ€bond calculations of the van der Waals interactions between Ï€ systems: The ethylene dimer. Journal of Chemical Physics, 1975, 62, 3326-3339.	3.0	59
43	Lattice dynamics of solid N2 with an ab initio intermolecular potential. Journal of Chemical Physics, 1980, 73, 5305-5309.	3.0	56
44	Scattering resonances in bimolecular collisions between NO radicals and H2 challenge the theoretical gold standard. Nature Chemistry, 2018, 10, 435-440.	13.6	56
45	New COâ€“CO interaction potential tested by rovibrational calculations. Journal of Chemical Physics, 2005, 122, 054306.	3.0	54
46	Ab initio Studies of long range interactions between ethylene molecules in the multipole expansion. Theoretica Chimica Acta, 1977, 46, 39-62.	0.8	53
47	Unambiguous assignment of the van der Waals modes of benzeneâ€“Ar by analysis of the rotationally resolved UVâ€spectra and comparison with multidimensional calculations. Journal of Chemical Physics, 1996, 104, 882-898.	3.0	53
48	Quantitative characterization of the (D2O)3 torsional manifold by terahertz laser spectroscopy and theoretical analysis. Journal of Chemical Physics, 1999, 110, 4369-4381.	3.0	53
49	DYNAMICS OF CO IN AMORPHOUS WATER-ICE ENVIRONMENTS. Astrophysical Journal, 2014, 781, 16.	4.5	52
50	Scattering resonances in slow NH3â€“He collisions. Journal of Chemical Physics, 2012, 136, 074301.	3.0	51
51	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
52	Imaging quantum stereodynamics through Fraunhofer scattering of NO radicals with rare-gas atoms. Nature Chemistry, 2017, 9, 226-233.	13.6	50
53	Ab initio potential energy surfaces of Arâ€“NH3 for different NH3 umbrella angles. Journal of Chemical Physics, 1991, 94, 491-500.	3.0	49
54	Quantitative characterization of the water trimer torsional manifold by terahertz laser spectroscopy and theoretical analysis. II. (H2O)3. Journal of Chemical Physics, 1999, 111, 7789-7800.	3.0	49

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55	Ab InitioPotential Energy Surface and Infrared Spectrum of the Neâ‹¯CO Complex. Journal of Physical Chemistry A, 1997, 101, 4690-4698.	2.5	48
56	Abinitiodescription of large amplitude motions in solid N2. II. Librons in the Î²â€phase and the Î±â€“Î² phase transition. Journal of Chemical Physics, 1984, 81, 3658-3665.	3.0	47
57	Magnetic coupling and dynamics in solid Î± and Î²â€O2. I. An ab initio theoretical approach. Journal of Chemical Physics, 1987, 86, 3583-3596.	3.0	45
58	Infrared spectra of the van der Waals molecule (N2)2. Molecular Physics, 1985, 55, 11-32.	1.7	42
59	Ab initio potential energy surfaces of Arâ€“H2O and Arâ€“D2O. Journal of Chemical Physics, 1991, 94, 8096-8104.	3.0	41
60	Infrared spectroscopy and ab initio potential energy surface for Neâ€“C2H2 and Neâ€“C2HD complexes. Journal of Chemical Physics, 1998, 109, 8968-8979.	3.0	41
61	Quantum calculation of vibrational states in the anilineâ€“argon van der Waals cluster. Journal of Chemical Physics, 1993, 98, 2709-2719.	3.0	40
62	Terahertz vibrationâ€“rotationâ€“tunneling spectroscopy of water clusters in the translational band region of liquid water. Journal of Chemical Physics, 2001, 114, 3994-4004.	3.0	40
63	Ab initio computed diabatic potential energy surfaces of OHâ€“HCl. Journal of Chemical Physics, 2005, 122, 244325.	3.0	40
64	Hartreeâ€“Fockâ€“Slaterâ€“LCAO calculations on the Cu(II) bis(dithiocarbamate) complex; magnetic coupling parameters and optical spectrum. Journal of Chemical Physics, 1980, 73, 1306-1312.	3.0	39
65	Ab initio description of large amplitude motions in solid N2. I. Librons in the ordered Î± and Î³ phases. Journal of Chemical Physics, 1984, 81, 3648-3657.	3.0	39
66	The O2â€“O2 dimer: Magnetic coupling and spectrum. Journal of Chemical Physics, 1987, 87, 5346-5360.	3.0	39
67	Lattice dynamics of the ethylene crystal with interaction potentials fromabinitiocalculations. Journal of Chemical Physics, 1978, 69, 5288-5300.	3.0	38
68	The nature of monomer inversion in the ammonia dimer. Journal of Chemical Physics, 1994, 101, 8443-8454.	3.0	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.	2.8	38
70	Cold and ultracold NH-NH collisions in magnetic fields. Physical Review A, 2011, 83, .	2.5	38
71	Vibration and rotation of CO in C60 and predicted infrared spectrum. Journal of Chemical Physics, 1996, 104, 832-847.	3.0	37
72	Determining the nature of quantum resonances by probing elastic and reactive scattering in cold collisions. Nature Chemistry, 2021, 13, 94-98.	13.6	37

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73	High-Resolution Imaging of Velocity-Controlled Molecular Collisions Using Counterpropagating Beams. Physical Review Letters, 2014, 113, 263202.	7.8	36
74	Higher Energy States in the CO Dimer:â€‰ Millimeter-Wave Spectra and Rovibrational Calculations. Journal of Physical Chemistry A, 2007, 111, 12238-12247.	2.5	35
75	Ab initio description of large amplitude motions in solid N2. III. Libronâ€“phonon coupling. Journal of Chemical Physics, 1984, 81, 4118-4126.	3.0	34
76	Resonances in rotationally inelastic scattering of NH3 and ND3 with H2. Journal of Chemical Physics, 2015, 143, 044312.	3.0	34
77	Rotationally inelastic scattering of OH by molecular hydrogen: Theory and experiment. Journal of Chemical Physics, 2015, 142, 204310.	3.0	34
78	The van der Waals rovibrational states of the Arâ€“NH3 dimer. Journal of Chemical Physics, 1991, 94, 501-510.	3.0	33
79	Transformation Properties of Antisymmetric Spin Eigenfunctions under Linear Mixing of the Orbitals. Journal of Chemical Physics, 1972, 57, 2498-2505.	3.0	32
80	Observation of correlated excitations in bimolecular collisions. Nature Chemistry, 2018, 10, 469-473.	13.6	32
81	Vibrational overtones in the electronic ground state of the benzene-Ar complex: A combined experimental and theoretical analysis. Journal of Chemical Physics, 1998, 108, 8408-8417.	3.0	31
82	Nearâ€infrared spectrum and rotational predissociation dynamics of the Heâ€“HF complex from an ab initio symmetryâ€adapted perturbation theory potential. Journal of Chemical Physics, 1994, 101, 2825-2835.	3.0	30
83	Near dissociation states for H₂⁺â€“He on MRCI and FCI potential energy surfaces. Physical Chemistry Chemical Physics, 2019, 21, 24976-24983.	2.8	30
84	Symmetry-adapted perturbation theory of nonadditive three-body interactions in van der Waals molecules. II. Application to the Ar2â€“HF interaction. Journal of Chemical Physics, 1998, 108, 579-589.	3.0	29
85	Water trimer torsional spectrum from accurate ab initio and semiempirical potentials. Journal of Chemical Physics, 2008, 128, 014302.	3.0	29
86	O2â^'O2 and O2â^'N2 collision-induced absorption mechanisms unravelled. Nature Chemistry, 2018, 10, 549-554.	13.6	29
87	Spectrum and vibrational predissociation of the HF dimer. I. Bound and quasibound states. Journal of Chemical Physics, 2003, 119, 277-285.	3.0	28
88	Resolving rainbows with superimposed diffraction oscillations in NO + rare gas scattering: experiment and theory. New Journal of Physics, 2015, 17, 055019.	2.9	28
89	The infrared photodissociation spectra and the internal mobility of SF6, SiF4, and SiH4dimers. Journal of Chemical Physics, 1990, 92, 2837-2847.	3.0	27
90	Overtone vibrational spectroscopy in H2-H2O complexes: A combined high level theoretical ab initio, dynamical and experimental study. Journal of Chemical Physics, 2012, 137, 084301.	3.0	27

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91	Three-Dimensional Ab Initio Potential Energy Surface for Hâ€“CO(XÌƒ²Aâ€²). Journal of Physical Chemistry A, 2013, 117, 7571-7579.	2.5	27
92	The interaction of OH(X2Î) with H2: Ab initio potential energy surfaces and bound states. Journal of Chemical Physics, 2014, 141, 174309.	3.0	26
93	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
94	Fineâ€structure spectrum of O2â€“rare gas van der Waals molecules. Journal of Chemical Physics, 1983, 79, 1170-1175.	3.0	25
95	Lattice dynamics of Î±â€CO from an ab initio potential. Journal of Chemical Physics, 1991, 94, 8402-8407.	3.0	25
96	Potential energy surface and bound states of the NH3â€“Ar and ND3â€“Ar complexes. Journal of Chemical Physics, 2014, 141, 224303.	3.0	25
97	Quantifying the interplay between fine structure and geometry of an individual molecule on a surface. Physical Review B, 2021, 103, .	3.2	25
98	Ab initio Studies of long range interactions between ethylene molecules in the multipole expansion. Theoretica Chimica Acta, 1977, 46, 39-62.	0.8	24
99	Pseudorotation tunneling in several water trimer isotopomers. Journal of Chemical Physics, 1999, 110, 823-831.	3.0	24
100	Bound states of the OH(Î2)â€“HCl complex on ab initio diabatic potentials. Journal of Chemical Physics, 2009, 131, 124307.	3.0	24
101	Resonances in rotationally inelastic scattering of OH(X2Î) with helium and neon. Journal of Chemical Physics, 2012, 136, 144308.	3.0	24
102	Scattering of NH3 and ND3 with rare gas atoms at low collision energy. Journal of Chemical Physics, 2015, 143, 184303.	3.0	24
103	Interaction of H₂O with CO: potential energy surface, bound states and scattering calculations. Physical Chemistry Chemical Physics, 2018, 20, 5469-5477.	2.8	24
104	Characterization of methanol as a magnetic field tracer in star-forming regions. Nature Astronomy, 2018, 2, 145-150.	10.1	23
105	The NH3 umbrella motion in the Arî—¸NH3 dimer. Chemical Physics, 1992, 165, 47-55.	1.9	22
106	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
107	Cold Collisions in a Molecular Synchrotron. Physical Review Letters, 2018, 120, 033402.	7.8	22
108	Stark effect and dipole moments of the ammonia dimer in different vibrationâ€“rotationâ€“tunneling states. Journal of Chemical Physics, 1996, 104, 3898-3906.	3.0	20

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109	State-to-state scattering of highly vibrationally excited NO at broadly tunable energies. Nature Chemistry, 2020, 12, 528-534.	13.6	20
110	Differential cross sections for rotational excitation of NH3 by collisions with Ar and He: Close coupling results and comparison with experiment. Journal of Chemical Physics, 1996, 105, 3079-3088.	3.0	19
111	The 583.2 GHz torsional hot-band of (D2O)3. Journal of Chemical Physics, 2001, 114, 3988-3993.	3.0	19
112	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
113	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
114	Rotationally inelastic scattering of ND₃with H₂as a probe of the intermolecular potential energy surface. Molecular Physics, 2015, 113, 3925-3933.	1.7	18
115	QUANTUM CALCULATION OF INELASTIC CO COLLISIONS WITH H. II. PURE ROTATIONAL QUENCHING OF HIGH ROTATIONAL LEVELS. Astrophysical Journal, 2015, 811, 27.	4.5	18
116	High-resolution spectroscopy of 4-fluorostyrene-rare gas van der Waals complexes: Results and comparison with theoretical calculations. Journal of Chemical Physics, 1998, 108, 1836-1850.	3.0	17
117	Rotational Spectroscopy of the NH₃â€“H₂ Molecular Complex. Astrophysical Journal, 2017, 838, 27.	4.5	17
118	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
119	Magnetic coupling and dynamics in solid Î± and Î²â€O2. II. Prediction of magnetic field effects. Journal of Chemical Physics, 1987, 86, 3597-3601.	3.0	16
120	Is the NH3â€“NH3riddle solved?. Faraday Discussions, 1994, 97, 43-55.	3.2	16
121	Method for the ab initio calculation of intermolecular potentials of ionic clusters: Test on Rgâ€“CO+, Rg=He, Ne, Ar. Journal of Chemical Physics, 2003, 118, 1110-1118.	3.0	16
122	Hyperfine interactions and internal rotation in methanol. Journal of Chemical Physics, 2016, 145, 244301.	3.0	16
123	Communication: Multiple-property-based diabatization for open-shell van der Waals molecules. Journal of Chemical Physics, 2016, 144, 121101.	3.0	16
124	Imaging diffraction oscillations for inelastic collisions of NO radicals with He and D2. Journal of Chemical Physics, 2017, 147, 013918.	3.0	16
125	Intramonomer correlation contributions to first-order exchange nonadditivity in trimers. Journal of Chemical Physics, 2000, 112, 3159-3169.	3.0	14
126	Rotational study of the NH3â€“CO complex: Millimeter-wave measurements and ab initio calculations. Journal of Chemical Physics, 2015, 142, 114308.	3.0	14

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127	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
128	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
129	Direct observation of product-pair correlations in rotationally inelastic collisions of ND₃ with D₂. Physical Chemistry Chemical Physics, 2019, 21, 14033-14041.	2.8	14
130	The waterâ€“carbon monoxide dimer: new infrared spectra, ab initio rovibrational energy level calculations, and an interesting in-termolecular mode. Physical Chemistry Chemical Physics, 2019, 21, 14911-14922.	2.8	14
131	Transformation properties of many-electron wave functions with special attention to the relation between pair-correlated DODS and configuration interaction. International Journal of Quantum Chemistry, 1974, 8, 715-732.	2.0	13
132	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
133	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
134	Photodissociation of the methaneâ€“argon complex. I.Ab initiointermolecular potential depending on the methane vibrational coordinates. Journal of Chemical Physics, 2002, 117, 7551-7561.	3.0	13
135	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
136	Ab initio potential-energy surface and rovibrational states of the HCNâ€“HCl complex. Journal of Chemical Physics, 2006, 124, 204315.	3.0	13
137	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
138	Ab initio potential and rotational spectra of the COâ€“N2 complex. Journal of Chemical Physics, 2018, 148, 044313.	3.0	13
139	Molecular square dancing in CO-CO collisions. Science, 2020, 369, 307-309.	12.6	13
140	Potential energy surface and bound states of the H2Oâ€“HF complex. Journal of Chemical Physics, 2020, 153, 214301.	3.0	13
141	Dynamical and optical properties of the ethylene crystal: Selfâ€consistent phonon calculations using an â€˜ab initioâ€™â€™ intermolecular potential. Journal of Chemical Physics, 1981, 75, 1451-1458.	3.0	12
142	Vibron band structure in chlorinated benzene crystals: Lattice dynamics calculations and Raman spectra of 1,2,4,5â€tetrachlorobenzene. Journal of Chemical Physics, 1988, 89, 4023-4034.	3.0	12
143	QUANTUM CALCULATION OF INELASTIC CO COLLISIONS WITH H. III. RATE COEFFICIENTS FOR RO-VIBRATIONAL TRANSITIONS. Astrophysical Journal, 2015, 813, 96.	4.5	12
144	Simulating rotationally inelastic collisions using a direct simulation Monte Carlo method. Molecular Physics, 2015, 113, 3972-3978.	1.7	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.	2.5	11
146	Quantum scattering calculations for ro-vibrational de-excitation of CO by hydrogen atoms. Journal of Chemical Physics, 2015, 142, 204303.	3.0	11
147	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
148	Paraâ€•ortho hydrogen conversion: Solving a 90â€•year old mystery. Natural Sciences, 2021, 1, e10002.	2.1	11
149	Rotational study of the CH4â€“CO complex: Millimeter-wave measurements and ab initio calculations. Journal of Chemical Physics, 2015, 143, 154303.	3.0	11
150	Glory scattering in deeply inelastic molecular collisions. Nature Chemistry, 2022, 14, 664-669.	13.6	11
151	Rotationally Inelastic Scattering of Quantum-State-Selected ND₃ withÂAr. Journal of Physical Chemistry A, 2015, 119, 5979-5987.	2.5	10
152	Direct Extraction of Alignment Moments from Inelastic Scattering Images. Journal of Physical Chemistry A, 2015, 119, 5925-5931.	2.5	10
153	Probing Scattering Resonances in (Ultra)Cold Inelastic NOâ€“He Collisions. Journal of Physical Chemistry A, 2016, 120, 4770-4777.	2.5	10
154	Using a direct simulation Monte Carlo approach to model collisions in a buffer gas cell. Journal of Chemical Physics, 2017, 146, 044302.	3.0	10
155	Rotationalâ€“vibrational resonance states. Physical Chemistry Chemical Physics, 2020, 22, 15081-15104.	2.8	10
156	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
157	The elusive S2 state, the S1/S2 splitting, and the excimer states of the benzene dimer. Journal of Chemical Physics, 2015, 142, 234306.	3.0	9
158	Near infrared overtone (νOH = 2 â†• 0) spectroscopy of Neâ€“H2O clusters. Journal of Chemical Physics, 2017, 146, 104204.	3.0	9
159	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
160	Fragmentation dynamics of the vibrationally excited ammoniaâ€“argon van der Waals complex. Journal of Chemical Physics, 1995, 103, 4138-4149.	3.0	8
161	Vibrational predissociation of the ND3-Ar Van der Waals complex: Comparison with NH3-Ar. Journal of Chemical Physics, 1997, 106, 9141-9154.	3.0	8
162	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

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163	Comment on â€œCommunication: Benzene dimerâ€”The free energy landscapeâ€•[J. Chem. Phys. 139, 201102 (2013)]. Journal of Chemical Physics, 2014, 140, 227101.	3.0	8
164	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
165	Diabatic states, nonadiabatic coupling, and the counterpoise procedure for weakly interacting open-shell molecules. Journal of Chemical Physics, 2018, 148, .	3.0	8
166	Vibrational spectroscopy of H2He+ and D2He+. Journal of Molecular Spectroscopy, 2021, 377, 111423.	1.2	8
167	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
168	Ab initio prediction of the vibration-rotation-tunneling spectrum of HClâ€“(H2O)2. Journal of Chemical Physics, 2001, 115, 3604-3613.	3.0	7
169	Ammonia dimer: extremely fluxional but still hydrogen bonded. Nature Communications, 2022, 13, 1470.	12.8	7
170	Mapping partial wave dynamics in scattering resonances by rotational de-excitation collisions. Nature Chemistry, 2022, 14, 538-544.	13.6	6
171	Hindered internal rotations in Van der Waals molecules and molecular crystals. International Journal of Quantum Chemistry, 1983, 23, 1091-1100.	2.0	5
172	Nuclear spin/parity dependent spectroscopy and predissociation dynamics in νOH = 2 â†•0 overtone excited Neâ€“H2O clusters: Theory and experiment. Journal of Chemical Physics, 2017, 147, 214304.	3.0	5
173	Rovibrational laser jet-cooled spectroscopy of the NH₃â€“Ar complex in the Î½₂ umbrella region of NH₃: comparison between new infrared data and an ab initio calculated spectrum. Molecular Physics, 2018, 116, 3642-3655.	1.7	5
174	Correlations in rotational energy transfer for NOâ€“D2 inelastic collisions. Journal of Chemical Physics, 2020, 153, 064301.	3.0	5
175	Experimental and theoretical investigation of resonances in low-energy NOâ€“H2 collisions. Journal of Chemical Physics, 2020, 153, 244302.	3.0	5
176	Collisionâ€•induced spinâ€•orbit relaxation of highly vibrationally excited NO near 1 K. Natural Sciences, 2022, 2, e20210074.	2.1	5
177	Jahnâ€“Teller effect in van der Waals complexes; Arâ€“C6H6+ and Arâ€“C6D6+. Journal of Chemical Physics, 2004, 120, 10069-10083.	3.0	4
178	Rovibronic spectroscopy of the van der Waals complex Heâ€“HCl+. Molecular Physics, 2004, 102, 2285-2295.	1.7	4
179	Molecules in confinement in clusters, quantum solvents and matrices: general discussion. Faraday Discussions, 2018, 212, 569-601.	3.2	4
180	Intermolecular dynamics of NH₃-rare gas complexes in the Î½₂ umbrella region of NH₃ investigated by rovibrational laser jet-cooled spectroscopy and ab initio calculations. Physical Chemistry Chemical Physics, 2021, 23, 10864-10874.	2.8	4

#	Article	IF	Citations
181	Multi-channel distorted-wave Born approximation for rovibrational transition rates in molecular collisions. Journal of Chemical Physics, 2021, 155, 034105.	3.0	4
182	Correlated rotational excitations in NO-CO inelastic collisions. Journal of Chemical Physics, 0, , .	3.0	4
183	Calculation of exchange forces between molecules by application of the Hellmann-Feynman theorem. Molecular Physics, 1977, 33, 1367-1377.	1.7	3
184	Imaging inelastic scattering of CO with argon: polarization dependent differential cross sections. Physical Chemistry Chemical Physics, 2019, 21, 9200-9211.	2.8	3
185	Ab initio potential energy surface and microwave spectrum of the NH3â€“N2 van der Waals complex. Journal of Chemical Physics, 2020, 152, 234304.	3.0	3
186	Rotational spectroscopy and bound state calculations of deuterated NH3â€“H2 van der Waals complexes. Journal of Molecular Spectroscopy, 2021, 377, 111442.	1.2	3
187	Ab initio study of the O3â€“N2 complex: Potential energy surface and rovibrational states. Journal of Chemical Physics, 2021, 155, 054308.	3.0	3
188	The Heâ€“H3+ complex. II. Infrared predissociation spectrum and energy term diagram. Journal of Chemical Physics, 2022, 156, 144308.	3.0	3
189	Comment on: The molecular symmetry group of the CO dimer and the assignments of the intermolecular vibrations, by: K.M.T. Yamada, J. Mol. Spectrosc. 254 (2009) 87. Journal of Molecular Spectroscopy, 2010, 259, 60-61.	1.2	2
190	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
191	Energy dependent parity-pair behavior in NO + He collisions. Journal of Chemical Physics, 2018, 149, 084306.	3.0	2
192	The Heâ€“H3+ complex. I. Vibration-rotation-tunneling states and transition probabilities. Journal of Chemical Physics, 2022, 156, 144307.	3.0	2
193	Vibration-Rotation-Tunneling Levels and Spectra of Van der Waals Molecules. , 2022, , 194-234.		2
194	Efficient computational methods for rovibrational transition rates in molecular collisions. Journal of Chemical Physics, 2022, 157, .	3.0	2
195	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
196	Rotational energy transfer in collisions of ammonia with rare gas atoms and H₂. Journal of Physics: Conference Series, 2017, 875, 102034.	0.4	0
197	Concluding remarks. Faraday Discussions, 2018, 212, 603-607.	3.2	0