# Gerrit C Groenenboom

List of Publications by Year
in descending order



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|---|---|---|---|
| 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 | Predictions of the Properties of Water from First Principles. Science, 2007, 315, 1249-1252. | 12.6 | 382 |
| 2 | Near-Threshold Inelastic Collisions Using Molecular Beams with a Tunable Velocity. Science, 2006, 313, 1617-1620. | 12.6 | 213 |
| 3 | 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 |
| 4 | Theoretical transition probabilities for the OH Meinel system. Journal of Chemical Physics, 2007, 126, 114314. | 3.0 | 126 |
| 5 | 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 |
| 6 | Imaging resonances in low-energy NO-He inelastic collisions. Science, 2015, 350, 787-790. | 12.6 | 115 |
| 7 | Quantum-State Resolved Bimolecular Collisions of Velocity-Controlled OH with NO Radicals. Science, 2012, 338, 1060-1063. | 12.6 | 114 |
| 8 | 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 |
| 9 | Update of the HITRAN collision-induced absorption section. Icarus, 2019, 328, 160-175. | 2.5 | 105 |
| 10 | 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 |
| 11 | Water Pair and Three-Body Potential of Spectroscopic Quality fromAb InitioCalculations. Physical Review Letters, 2000, 84, 4072-4075. | 7.8 | 102 |
| 12 | 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 |
| 13 | Vibrations, Tunneling, and Transition Dipole Moments in the Water Dimer. Journal of Physical Chemistry A, 2001, 105, 6212-6225. | 2.5 | 100 |
| 14 | Direct Measurement of the Radiative Lifetime of Vibrationally Excited OH Radicals. Physical Review Letters, 2005, 95, 013003. | 7.8 | 93 |
| 15 | The radiative lifetime of metastable CO (aÎ3, v=). Journal of Chemical Physics, 2007, 127, 221102. | 3.0 | 93 |
| 16 | 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 |
| 17 | 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 |
| 18 | Photoinduced Two-Body Loss of Ultracold Molecules. Physical Review Letters, 2019, 123, 123402. | 7.8 | 84 |

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| 19 | New applications of the genetic algorithm for the interpretation of high-resolution spectra. Canadian Journal of Chemistry, 2004, 82, 804-819. | 1.1 | 81 |
| 20 | 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 |
| 21 | Electronic Interaction Anisotropy between Atoms in Arbitrary Angular Momentum Statesâ€. Journal of Physical Chemistry A, 2004, 108, 8941-8948. | 2.5 | 75 |
| 22 | 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 |
| 23 | Imaging the onset of the resonance regime in low-energy NO-He collisions. Science, 2020, 368, 626-630. | 12.6 | 68 |
| 24 | Spin-flipping transitions in2Î£molecules induced by collisions with structureless atoms. Physical Review A, 2003, 67, . | 2.5 | 65 |
| 25 | 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 |
| 26 | Scattering resonances in bimolecular collisions between NO radicals and H2 challenge the theoretical gold standard. Nature Chemistry, 2018, 10, 435-440. | 13.6 | 56 |
| 27 | 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 |
| 28 | Three-dimensional ab initio potential energy surface for Heâ€“O2. Journal of Chemical Physics, 2000, 113, 9562-9566. | 3.0 | 52 |
| 29 | Scattering resonances in slow NH3â€“He collisions. Journal of Chemical Physics, 2012, 136, 074301. | 3.0 | 51 |
| 30 | 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><mml:r | 7.8 | 50 |
| 31 | Imaging quantum stereodynamics through Fraunhofer scattering of NO radicals with rare-gas atoms. Nature Chemistry, 2017, 9, 226-233. | 13.6 | 50 |
| 32 | Quasiclassical method for calculating the density of states of ultracold collision complexes. Physical Review A, 2019, 100, . | 2.5 | 50 |
| 33 | O(3PJ) Alignment from the Photodissociation of SO2at 193 nmâ€. Journal of Physical Chemistry A, 2004, 108, 7965-7976. | 2.5 | 49 |
| 34 | Time-Domain Measurement of Spontaneous Vibrational Decay of Magnetically Trapped NH. Physical Review Letters, 2008, 100, 083003. | 7.8 | 48 |
| 35 | Dynamic polarizabilities of rare-earth-metal atoms and dispersion coefficients for their interaction with helium atoms. Physical Review A, 2007, 75, . | 2.5 | 43 |
| 36 | State-to-state reaction probabilities for Hâ^ + H2, D2 collisions. Chemical Physics Letters, 1993, 209, 309-314. | 2.6 | 42 |

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| 37 | 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 |
| 38 | Ab initio computed diabatic potential energy surfaces of OHâ€“HCl. Journal of Chemical Physics, 2005, 122, 244325. | 3.0 | 40 |
| 39 | Cold and ultracold NH-NH collisions in magnetic fields. Physical Review A, 2011, 83, . | 2.5 | 38 |
| 40 | Scattering of Stark-decelerated OH radicals with rare-gas atoms. European Physical Journal D, 2011, 65, 189-198. | 1.3 | 38 |
| 41 | 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 |
| 42 | 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 |
| 43 | High-Resolution Imaging of Velocity-Controlled Molecular Collisions Using Counterpropagating Beams. Physical Review Letters, 2014, 113, 263202. | 7.8 | 36 |
| 44 | Dynamical calculations on the photoisomerization of small polyenes in a nonadiabatic formalism. Journal of Chemical Physics, 1987, 86, 4895-4909. | 3.0 | 35 |
| 45 | 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 |
| 46 | 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 |
| 47 | 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 |
| 48 | Photodissociation of singlet oxygen in the UV region. Physical Chemistry Chemical Physics, 2014, 16, 3305. | 2.8 | 33 |
| 49 | Observation of correlated excitations in bimolecular collisions. Nature Chemistry, 2018, 10, 469-473. | 13.6 | 32 |
| 50 | 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 |
| 51 | 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 |
| 52 | 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 |
| 53 | O2â¯O2 and O2â¯N2 collision-induced absorption mechanisms unravelled. Nature Chemistry, 2018, 10, 549-554. | 13.6 | 29 |
| 54 | Solving the discretized timeâ€independent SchrÃ¶dinger equation with the Lanczos procedure. Journal of Chemical Physics, 1990, 92, 4374-4379. | 3.0 | 28 |

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| 55 | Spectrum and vibrational predissociation of the HF dimer. I. Bound and quasibound states. Journal of Chemical Physics, 2003, 119, 277-285. | 3.0 | 28 |
| 56 | Resolving rainbows with superimposed diffraction oscillations in NO + rare gas scattering: experiment and theory. New Journal of Physics, 2015, 17, 055019. | 2.9 | 28 |
| 57 | Three-Dimensional Ab Initio Potential Energy Surface for Hâ€“CO(XÌƒ<sup>2</sup>Aâ€²). Journal of Physical Chemistry A, 2013, 117, 7571-7579. | 2.5 | 27 |
| 58 | Photodissociation Imaging of Diatomic Sulfur (S<sub>2</sub>). Journal of Physical Chemistry A, 2009, 113, 14995-15005. | 2.5 | 26 |
| 59 | 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 |
| 60 | 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 |
| 61 | Quantifying the interplay between fine structure and geometry of an individual molecule on a surface. Physical Review B, 2021, 103, . | 3.2 | 25 |
| 62 | Bound states of the OH(Î2)â€“HCl complex on ab initio diabatic potentials. Journal of Chemical Physics, 2009, 131, 124307. | 3.0 | 24 |
| 63 | Resonances in rotationally inelastic scattering of OH(X2Î) with helium and neon. Journal of Chemical Physics, 2012, 136, 144308. | 3.0 | 24 |
| 64 | 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 |
| 65 | Photolysis of NO2 at multiple wavelengths in the spectral region 200â€“205Ânm. European Physical Journal D, 2006, 38, 151-162. | 1.3 | 23 |
| 66 | Dynamics of OH(2Î)â€“He collisions in combined electric and magnetic fields. Faraday Discussions, 2009, 142, 127. | 3.2 | 23 |
| 67 | Characterization of methanol as a magnetic field tracer in star-forming regions. Nature Astronomy, 2018, 2, 145-150. | 10.1 | 23 |
| 68 | 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 |
| 69 | Vibrational predissociation in the HCl dimer. Journal of Chemical Physics, 2004, 120, 9487-9498. | 3.0 | 22 |
| 70 | The photodissociation dynamics of ozone at 193nm: An O(D21) angular momentum polarization study. Journal of Chemical Physics, 2006, 125, 133308. | 3.0 | 22 |
| 71 | Polarizabilities of Sc and Ti atoms and dispersion coefficients for their interaction with helium atoms. Physical Review A, 2005, 72, . | 2.5 | 21 |
| 72 | Photodissociation dynamics of the Aâ€‰Î£2+ state of SH and SD radicals. Journal of Chemical Physics, 2009, 130, 034307. | 3.0 | 21 |

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| 73 | Product pair correlation in CH<sub>3</sub>OH photodissociation at 157 nm: the OH + CH<sub>3</sub>channel. Physical Chemistry Chemical Physics, 2011, 13, 2350-2355. | 2.8 | 21 |
| 74 | 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 |
| 75 | 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 |
| 76 | Cold Collisions of OH(<sup>2</sup>Î) Molecules with He Atoms in External Fields. Journal of Physical Chemistry A, 2009, 113, 14670-14680. | 2.5 | 20 |
| 77 | Cold and ultracold NHâ€“NH collisions: The field-free case. Journal of Chemical Physics, 2011, 134, 124309. | 3.0 | 20 |
| 78 | State-to-state scattering of highly vibrationally excited NO at broadly tunable energies. Nature Chemistry, 2020, 12, 528-534. | 13.6 | 20 |
| 79 | 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 |
| 80 | 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 |
| 81 | 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 |
| 82 | 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 |
| 83 | 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 |
| 84 | QUANTUM CALCULATION OF INELASTIC CO COLLISIONS WITH H. II. PURE ROTATIONAL QUENCHING OF HIGH ROTATIONAL LEVELS. Astrophysical Journal, 2015, 811, 27. | 4.5 | 18 |
| 85 | Ab initiopotential-energy surface for the reaction Ca+HClâ†CaCl+H. Journal of Chemical Physics, 2005, 122, 204307. | 3.0 | 17 |
| 86 | 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 density-functional-theory study. Physical Review A, 2016, 93, . | 2.5 | 17 |
| 87 | 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 |
| 88 | Controlling the nature of a charged impurity in a bath of Feshbach dimers. Physical Review Research, 2020, 2, . | 3.6 | 17 |
| 89 | 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 |
| 90 | Electronic anisotropy between open shell atoms in first and second order perturbation theory. Journal of Chemical Physics, 2007, 126, 204306. | 3.0 | 16 |

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| 91 | 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 |
| 92 | Hyperfine interactions and internal rotation in methanol. Journal of Chemical Physics, 2016, 145, 244301. | 3.0 | 16 |
| 93 | Communication: Multiple-property-based diabatization for open-shell van der Waals molecules. Journal of Chemical Physics, 2016, 144, 121101. | 3.0 | 16 |
| 94 | Imaging diffraction oscillations for inelastic collisions of NO radicals with He and D2. Journal of Chemical Physics, 2017, 147, 013918. | 3.0 | 16 |
| 95 | Competition between photodetachment and photodissociation in O2â^'. Journal of Chemical Physics, 2003, 119, 8864-8872. | 3.0 | 15 |
| 96 | Photodissociation of the OD radical at 226 and 243 nm. Journal of Chemical Physics, 2003, 119, 9341-9343. | 3.0 | 15 |
| 97 | 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 |
| 98 | Photodissociation of vibrationally excited OH/OD radicals. Molecular Physics, 2008, 106, 557-572. | 1.7 | 15 |
| 99 | 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 |
| 100 | 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 |
| 101 | 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 |
| 102 | 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 |
| 103 | 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 |
| 104 | Spin-orbit relaxation of Cl(P1â^•22) and F(P1â^•22) in a gas of H2. Journal of Chemical Physics, 2007, 126, 184303. | 3.0 | 13 |
| 105 | (2+1)REMPI on molecular nitrogen through the 1Î£g+ (II)-state. Chemical Physics Letters, 2007, 435, 242-246. | 2.6 | 13 |
| 106 | State-to-State Differential Cross Sections for Inelastic Collisions of NO Radicals with para-H<sub>2</sub> and ortho-D<sub>2</sub>. Journal of Physical Chemistry A, 2017, 121, 7446-7454. | 2.5 | 13 |
| 107 | Lossy quantum defect theory of ultracold molecular collisions. Physical Review A, 2021, 104, . | 2.5 | 13 |
| 108 | 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 |

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| 109 | Heî—¸HF scattering cross sections from an ab initio SAPT potential: confrontation with experiment. Chemical Physics Letters, 1996, 263, 107-112. | 2.6 | 12 |
| 110 | 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 |
| 111 | Communication: Magnetic dipole transitions in the OH Aâ€‰2Î£+ â†•Xâ€‰2Î system. Journal of Chemical Physics, 2012, 137, 101102. | 3.0 | 12 |
| 112 | QUANTUM CALCULATION OF INELASTIC CO COLLISIONS WITH H. III. RATE COEFFICIENTS FOR RO-VIBRATIONAL TRANSITIONS. Astrophysical Journal, 2015, 813, 96. | 4.5 | 12 |
| 113 | Entrance Channel Effects in the Reaction of Aligned Ca(1P) with HCl. Journal of Physical Chemistry A, 1997, 101, 7558-7566. | 2.5 | 11 |
| 114 | Quantum scattering calculations for ro-vibrational de-excitation of CO by hydrogen atoms. Journal of Chemical Physics, 2015, 142, 204303. | 3.0 | 11 |
| 115 | Correlated energy transfer in rotationally and spinâ€“orbit inelastic collisions of NO(X<sup>2</sup>Î<sub>1/2</sub>, j = 1/2f) with O<sub>2</sub>(X<sup>3</sup>Î£<sub>g</sub><sup>â˜</sup>). Physical Chemistry Chemical Physics, 2018, 20, 12444-12453. | 2.8 | 11 |
| 116 | Paraâ€ortho hydrogen conversion: Solving a 90â€year old mystery. Natural Sciences, 2021, 1, e10002. | 2.1 | 11 |
| 117 | Glory scattering in deeply inelastic molecular collisions. Nature Chemistry, 2022, 14, 664-669. | 13.6 | 11 |
| 118 | Angular momentum polarisation in the O(<sup>1</sup>D) products of O<sub>2</sub>photolysis via the B state. Molecular Physics, 2010, 108, 1145-1157. | 1.7 | 10 |
| 119 | Producing translationally cold, ground-state CO molecules. Journal of Chemical Physics, 2011, 135, 114201. | 3.0 | 10 |
| 120 | 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 |
| 121 | Direct Extraction of Alignment Moments from Inelastic Scattering Images. Journal of Physical Chemistry A, 2015, 119, 5925-5931. | 2.5 | 10 |
| 122 | Probing Scattering Resonances in (Ultra)Cold Inelastic NOâ€“He Collisions. Journal of Physical Chemistry A, 2016, 120, 4770-4777. | 2.5 | 10 |
| 123 | Rotationalâ€“vibrational resonance states. Physical Chemistry Chemical Physics, 2020, 22, 15081-15104. | 2.8 | 10 |
| 124 | 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 |
| 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 | 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 |

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| 127 | 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:math> atoms. I. Interaction potential. Physical Review A, 2014, 90, . | 2.5 | 9 |
| 128 | A renormalized potential-following propagation algorithm for solving the coupled-channels equations. Journal of Chemical Physics, 2014, 141, 064102. | 3.0 | 9 |
| 129 | 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 |
| 130 | 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 |
| 131 | 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 |
| 132 | Correlated fine structure branching ratios arising from state-selected predissociation of ClO (A2Î3/2). Physical Chemistry Chemical Physics, 2009, 11, 4770. | 2.8 | 8 |
| 133 | Control and imaging of O(1D2) precession. Nature Chemistry, 2011, 3, 28-33. | 13.6 | 8 |
| 134 | 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 |
| 135 | Diabatic states, nonadiabatic coupling, and the counterpoise procedure for weakly interacting open-shell molecules. Journal of Chemical Physics, 2018, 148, . | 3.0 | 8 |
| 136 | Quantum spin systems versus Schroedinger operators: A case study in spontaneous symmetry breaking. SciPost Physics, 2020, 8, . | 4.9 | 8 |
| 137 | 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 |
| 138 | Ab initio prediction of the vibration-rotation-tunneling spectrum of HClâ€"(H2O)2. Journal of Chemical Physics, 2001, 115, 3604-3613. | 3.0 | 7 |
| 139 | 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 |
| 140 | Predissociation of the A2Î£+ (vâ€² = 3) state of the OH radical. Physical Chemistry Chemical Physics, 2009, 11, 4754. | 2.8 | 6 |
| 141 | Mapping partial wave dynamics in scattering resonances by rotational de-excitation collisions. Nature Chemistry, 2022, 14, 538-544. | 13.6 | 6 |
| 142 | Correlations in rotational energy transfer for NOâ€"D2 inelastic collisions. Journal of Chemical Physics, 2020, 153, 064301. | 3.0 | 5 |
| 143 | Experimental and theoretical investigation of resonances in low-energy NOâ€"H2 collisions. Journal of Chemical Physics, 2020, 153, 244302. | 3.0 | 5 |
| 144 | Collisionâ€induced spinâ€orbit relaxation of highly vibrationally excited NO near 1 K. Natural Sciences, 2022, 2, e20210074. | 2.1 | 5 |

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| 145 | Rovibronic spectroscopy of the van der Waals complex Heâ€“HCl+. Molecular Physics, 2004, 102, 2285-2295. | 1.7 | 4 |
| 146 | Cold magnetically trapped2Dgscandium atoms. II. Scattering dynamics. Physical Review A, 2014, 90, . | 2.5 | 4 |
| 147 | Time-dependent density-functional-theory study of the suppressed tunneling ionization of vanadium. Physical Review A, 2016, 94, . | 2.5 | 4 |
| 148 | Multi-channel distorted-wave Born approximation for rovibrational transition rates in molecular collisions. Journal of Chemical Physics, 2021, 155, 034105. | 3.0 | 4 |
| 149 | Correlated rotational excitations in NO-CO inelastic collisions. Journal of Chemical Physics, 0, , . | 3.0 | 4 |
| 150 | Discrete variational quantum reactive scattering method with optimal distorted waves. I. Theory. Journal of Chemical Physics, 1998, 108, 5670-5676. | 3.0 | 3 |
| 151 | Raman association of H2 in the early universe. Faraday Discussions, 2006, 133, 43. | 3.2 | 3 |
| 152 | Laser ionisation detection of O(<sup>3</sup>P<sub>j</sub>) atoms in the VUV; application to photodissociation of O<sub>2</sub>. Molecular Physics, 2022, 120, . | 1.7 | 3 |
| 153 | Ab initio study of the reactivity of ultracold RbSr + RbSr collisions. New Journal of Physics, 2022, 24, 055001. | 2.9 | 3 |
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