David C Clary

List of Publications by Citations

349 papers	15,437 citations	60 h-index	107 g-index
375 ext. papers	16,112 ext. citations	4.9 avg, IF	6.62 L-index

#	Paper	IF	Citations
349	Definition of the hydrogen bond (IUPAC Recommendations 2011). *Pure and Applied Chemistry*, **2011**, 83, 1637-1641	2.1	1111
348	Defining the hydrogen bond: An account (IUPAC Technical Report). *Pure and Applied Chemistry*, **2011**, 83, 1619-1636	2.1	738
347	Characterization of a cage form of the water hexamer. *Nature*, **1996**, 381, 501-503	50.4	566
346	The Water Dipole Moment in Water Clusters. *Science*, **1997**, 275, 814-7	33.3	556
345	Potential optimized discrete variable representation. *Chemical Physics Letters*, **1992**, 190, 225-230	2.5	517
344	Quantum scattering calculations on chemical reactions. *Annual Review of Physical Chemistry*, **2003**, 54, 493-529	15.7	340
343	Structure of Water Clusters. The Contribution of Many-Body Forces, Monomer Relaxation, and Vibrational Zero-Point Energy. *The Journal of Physical Chemistry*, **1996**, 100, 18014-18022		233
342	Fast Chemical Reactions: Theory Challenges Experiment. *Annual Review of Physical Chemistry*, **1990**, 41, 61-90	15.7	181
341	Rates of chemical reactions dominated by long-range intermolecular forces. *Molecular Physics*, **1984**, 53, 3-21	1.7	177
340	Predicting catalysis: understanding ammonia synthesis from first-principles calculations. *Journal of Physical Chemistry B*, **2006**, 110, 17719-35	3.4	168
339	Quantum reactive scattering of four-atom reactions with nonlinear geometry: OH+H2->H2O+H. *Journal of Chemical Physics*, **1991**, 95, 7298-7310	3.9	164
338	Four-Atom Reaction Dynamics. *The Journal of Physical Chemistry*, **1994**, 98, 10678-10688		142
337	Calculations of rate constants for ion-molecule reactions using a combined capture and centrifugal sudden approximation. *Molecular Physics*, **1985**, 54, 605-618	1.7	135
336	Sticking of hydrogen chloride and chlorine hydroxide to ice: a computational study. *The Journal of Physical Chemistry*, **1992**, 96, 7079-7088		133
335	Quantum theory of chemical reaction dynamics. *Science*, **1998**, 279, 1879-82	33.3	131
334	Calculations of the tunneling splittings in water dimer and trimer using diffusion Monte Carlo. *Journal of Chemical Physics*, **1995**, 102, 7817-7829	3.9	125
333	Combining ab initio computations, neural networks, and diffusion Monte Carlo: An efficient method to treat weakly bound molecules. *Journal of Chemical Physics*, **1996**, 105, 7597-7604	3.9	122

332	Interaction of HCl with water clusters: (H2O)nHCl, n = 1-3. *The Journal of Physical Chemistry*, **1995**, 99, 14323-14333		115
331	Ab Initio Calculations on Uracil□Water. *Journal of Physical Chemistry A*, **1999**, 103, 1611-1618	2.8	111
330	Quantum scattering calculations on the OH+H2(v=0,1), OH+D2, and OD+H2 reactions. *Journal of Chemical Physics*, **1992**, 96, 3656-3665	3.9	107
329	Application of hyperspherical coordinates to four-atom reactive scattering: H2+CN->H+HCN. *Journal of Chemical Physics*, **1990**, 92, 4178-4190	3.9	106
328	A quantum model Hamiltonian to treat reactions of the type X+YCZ3->XY+CZ3: Application to O(3P)+CH4->OH+CH3. *Journal of Chemical Physics*, **2000**, 112, 1859-1867	3.9	103
327	The dynamics of the reaction OH + D2 -> HOD + D: Crossed beam experiments and quantum mechanical scattering calculations on ab initio potential energy surfaces. *Chemical Physics*, **1996**, 207, 389-409	2.3	102
326	Quantum dynamical stereochemistry of atom□diatom reactions. *Journal of Chemical Physics*, **1997**, 106, 4509-4521	3.9	100
325	Temperature dependence of rate coefficients for reactions of ions with dipolar molecules. *Chemical Physics Letters*, **1985**, 119, 320-326	2.5	98
324	Quantum and quasiclassical calculations on the OH+CO->CO2+H reaction. *Journal of Chemical Physics*, **1993**, 99, 4578-4589	3.9	97
323	Three-body effects on molecular properties in the water trimer. *Journal of Chemical Physics*, **1995**, 103, 8924-8930	3.9	95
322	Formation of molecular hydrogen on a graphite surface via an Eley□Rideal mechanism. *Chemical Physics Letters*, **2000**, 319, 303-308	2.5	93
321	New Potential Energy Function for Four-Atom Reactions. Application to OH + H2. *Journal of Physical Chemistry A*, **1998**, 102, 9631-9637	2.8	93
320	Rydberg□Klein□Rees inversion of high resolution van der Waals infrared spectra: An intermolecular potential energy surface for Ar+HF (v=1). *Journal of Chemical Physics*, **1989**, 90, 4855-4864	3.9	92
319	Mechanisms for supercollisions. *Faraday Discussions*, **1995**, 102, 423	3.6	90
318	Using quantum rotational polarization moments to describe the stereodynamics of the H+D2(v=0,j=0)->HD(v?,j?)+D reaction. *Journal of Chemical Physics*, **1998**, 108, 3142-3153	3.9	89
317	Quantum theory of planar four-atom reactions. *Journal of Chemical Physics*, **1994**, 100, 402-422	3.9	89
316	Interstellar carbon chemistry: Reaction rates of neutral atomic carbon with organic molecules. *Astrophysical Journal*, **1994**, 422, 416	4.7	89
315	Mode selective chemistry in the reactions of OH with HBr and HCl. *Journal of Chemical Physics*, **1994**, 101, 3704-3714	3.9	88

314	Photodetachment of electrons from dipolar anions. *The Journal of Physical Chemistry*, **1988**, 92, 3173-3181		88
313	Quantum calculations on the rate constant for the O + OH reaction. *Chemical Physics Letters*, **1984**, 112, 346-350	2.5	85
312	Time-Dependent Quantum Mechanical Calculations on the Formation of Molecular Hydrogen on a Graphite Surface via an Eley□Rideal Mechanism□ *Journal of Physical Chemistry A*, **2001**, 105, 2173-2182	2.8	83
311	Quantum theory of four-atom reactions using arrangement channel hyperspherical coordinates: Formulation and application to OH+H2<->H2O+H. *Journal of Chemical Physics*, **1997**, 107, 8975-8984	3.9	81
310	Ab initio and diffusion Monte Carlo study of uracil□water, thymine□water, cytosine□water, and cytosine□(water)2. *Physical Chemistry Chemical Physics*, **2000**, 2, 1281-1290	3.6	81
309	Quantum scattering and quasi-classical trajectory calculations for the H2+OH?H2O+H reaction on a new potential surface. *Physical Chemistry Chemical Physics*, **2000**, 2, 693-700	3.6	81
308	Quantum dynamics of the Walden inversion reaction Cl□CH3Cl->ClCH3+Cl□ *Journal of Chemical Physics*, **1997**, 106, 575-583	3.9	80
307	Tunneling dynamics in water tetramer and pentamer. *Journal of Chemical Physics*, **1996**, 105, 6626-6633	3.9	77
306	Quantum study of vibrational excitation in the three-dimensional collisions of CO2 with rare gas atoms. *Journal of Chemical Physics*, **1981**, 75, 209-219	3.9	77
305	C + C2H2: A Key Reaction in Interstellar Chemistry. *Journal of Physical Chemistry A*, **2002**, 106, 5541-5552	2.8	73
304	Calculation of the intermolecular bound states for water dimer. *Journal of Chemical Physics*, **1994**, 101, 3603-3609	3.9	72
303	Kinetic isotope effects in the Mu+H2 and Mu+D2 reactions: Accurate quantum calculations for the collinear reactions and variational transition state theory predictions for one and three dimensions. *Journal of Chemical Physics*, **1982**, 76, 4986-4995	3.9	71
302	Quantum scattering calculations on the CH4+OH->CH3+H2O reaction. *Journal of Chemical Physics*, **1994**, 101, 5756-5771	3.9	70
301	Calculation of the electronic spectrum for Ar□OH. *Journal of Chemical Physics*, **1990**, 93, 3367-3378	3.9	70
300	Slit jet infrared spectroscopy of NeHF complexes: Internal rotor and J-dependent predissociation dynamics. *Journal of Chemical Physics*, **1989**, 91, 722-731	3.9	68
299	Calculation of van der Waals spectra for H2HF, D2HF, and H2DF. *Journal of Chemical Physics*, **1990**, 93, 6334-6349	3.9	68
298	State-selected vibrational relaxation rates for highly vibrationally excited oxygen molecules. *Journal of Chemical Physics*, **1995**, 102, 9544-9556	3.9	65
297	Calculation of vibration□otation spectra for rare gas□HCl complexes. *Journal of Chemical Physics*, **1989**, 90, 7000-7013	3.9	64

296	Quantum dynamics of the O(3P)+CH4->CH3+OH reaction. *Physical Chemistry Chemical Physics*, **1999**, 1, 1173-1179	3.6	63
295	Theoretical Study of the Cage Water Hexamer Structure. *Journal of Physical Chemistry A*, **1997**, 101, 6813-6819	2.8	62
294	Bond-selected reaction of HOD with H atoms. *Chemical Physics Letters*, **1992**, 192, 34-40	2.5	62
293	Chemical reactions dominated by long-range intermolecular forces. *Faraday Discussions of the Chemical Society*, **1987**, 84, 333		62
292	Rate constants for the reactions of ions with dipolar polyatomic molecules. *Journal of the Chemical Society, Faraday Transactions 2*, **1987**, 83, 139		62
291	Ab initio rate constants from hyperspherical quantum scattering: application to H + CH4 --> H2 + CH3. *Journal of Chemical Physics*, **2004**, 120, 2308-18	3.9	61
290	Rate coefficients of the reactions of ions with polar molecules at interstellar temperatures. *Astrophysical Journal*, **1985**, 296, L31	4.7	61
289	Quantum scattering calculations on H2O+H->H2+OH and isotopes: Rotational distributions and cross sections. *Journal of Chemical Physics*, **1993**, 99, 7774-7786	3.9	60
288	Ultra-low temperature kinetics of neutral□neutral reactions: New experimental and theoretical results for OH+HBr between 295 and 23 K. *Journal of Chemical Physics*, **1994**, 101, 1748-1751	3.9	60
287	Stimulated emission pumping of van der Waals vibrations in the ground electronic state of OH?Ar. *Chemical Physics Letters*, **1991**, 178, 301-310	2.5	60
286	Rate constant calculations on fast diatom□diatom reactions. *Journal of the Chemical Society, Faraday Transactions*, **1991**, 87, 1667-1679		60
285	Nucleophilic displacement as a function of hydration number and temperature: rate constants and product distributions for OD-(D2O)0,1,2,3 + CH3Cl at 200-500 K. *Journal of the American Chemical Society*, **1986**, 108, 3142-3143	16.4	60
284	A multifaceted approach to hydrogen storage. *Physical Chemistry Chemical Physics*, **2011**, 13, 16955-72	3.6	58
283	Rate constants for chemical reactions of radicals at low temperatures. *Journal of the Chemical Society, Faraday Transactions*, **1993**, 89, 2185		58
282	Quantum simulation of the benzene-water complex. *Molecular Physics*, **1996**, 88, 33-52	1.7	58
281	Quantum-mechanical calculations on termolecular association reactions XY+Z+M->XYZ+M: Application to ozone formation. *Journal of Chemical Physics*, **2002**, 117, 1660-1672	3.9	57
280	A comparison of conventional and rigid body diffusion Monte Carlo techniques. Application to water dimer. *Chemical Physics Letters*, **1994**, 228, 547-554	2.5	57
279	Configuration-interaction-Hylleraas calculations on one-positron atomic systems. *Journal of Physics B: Atomic and Molecular Physics*, **1976**, 9, 3115-3129		57

278	Temperature dependence of the rate constant for the Cl+CH3Br reaction down to 23 K. *Journal of Chemical Physics*, **1997**, 107, 1021-1024	3.9	56
277	Influence of surface defects on the adsorption of HCl on ice. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 2763-2767		56
276	A study of HOCO resonances in the OH+CO->CO2+H reaction. *Journal of Chemical Physics*, **1994**, 101, 2779-2784	3.9	56
275	Rovibrational spectra of open-shell van der Waals complexes: Ar–OH(X 2). *Journal of Chemical Physics*, **1991**, 94, 4149-4160	3.9	56
274	Calculation of the far-infrared spectra for (HF)2, (HCL)2 and (HBr)2. *Chemical Physics Letters*, **1991**, 187, 345-353	2.5	55
273	Existence of a bound state for the three-dimensional IHI molecule on a purely repulsive potential energy surface. *Chemical Physics Letters*, **1983**, 94, 81-84	2.5	55
272	Recent advances in quantum scattering calculations on polyatomic bimolecular reactions. *Chemical Society Reviews*, **2017**, 46, 7625-7649	58.5	53
271	Quantum reactive scattering of H + hydrocarbon reactions. *Physical Chemistry Chemical Physics*, **2006**, 8, 917-25	3.6	53
270	Zero temperature quantum properties of small protonated water clusters (H2O)nH+ (n=1–8). *Journal of Chemical Physics*, **2003**, 119, 10048-10062	3.9	52
269	Vibrational relaxation of N2 by collision with He atoms. *Journal of Chemical Physics*, **1986**, 84, 3788-3797	3.9	52
268	Quantum dynamics of chemical reactions. *Science*, **2008**, 321, 789-91	33.3	51
267	H-densities: a new concept for hydrated molecules. *Accounts of Chemical Research*, **2000**, 33, 441-7	24.3	51
266	Solvation of hydrogen halides on the surface of ice. *Faraday Discussions*, **1995**, 100, 309	3.6	51
265	Time-dependent wave-packet studies on the sticking of HCl to an ice surface. *Journal of Chemical Physics*, **1996**, 104, 5663-5673	3.9	51
264	Vibrational and rotational effects in the Cl+HOD<->HCl+OD reaction. *Journal of Chemical Physics*, **1994**, 100, 3556-3567	3.9	51
263	Refinement of the OH A 2+(v=0)+Ar intermolecular potential energy surface. *Journal of Chemical Physics*, **1993**, 98, 9320-9334	3.9	50
262	Coupled-channel calculations on energy transfer, photochemistry, and reactions of polyatomic molecules. *The Journal of Physical Chemistry*, **1987**, 91, 1718-1727		50
261	Theoretical studies on bimolecular reaction dynamics. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 12649-53	11.5	49

260	Reduced dimensionality quantum dynamics of Cl + CH4 --> HCl + CH3 on an ab initio potential. *Physical Chemistry Chemical Physics*, **2007**, 9, 933-43	3.6	49
259	Quantum free energies of the conformers of glycine on an ab initio potential energy surface. *Physical Chemistry Chemical Physics*, **2004**, 6, 2563	3.6	49
258	Ab initio rate constants from hyperspherical quantum scattering: application to H+C2H6 and H+CH3OH. *Journal of Chemical Physics*, **2004**, 121, 6809-21	3.9	46
257	Quantum scattering on SN2 reactions: Influence of azimuthal rotations. *Journal of Chemical Physics*, **1998**, 109, 8200-8217	3.9	46
256	Rate constant calculations on the C++HCl reaction. *Journal of Chemical Physics*, **1989**, 90, 7216-7228	3.9	46
255	A new theory for vibrational and rotational energy transfer in the collisions of atoms with symmetric top molecules. *Journal of Chemical Physics*, **1984**, 81, 4466-4473	3.9	46
254	Quantum-mechanical calculations on pressure and temperature dependence of three-body recombination reactions: application to ozone formation rates. *Journal of Chemical Physics*, **2004**, 120, 2700-7	3.9	45
253	Ab initio computation of vibrational relaxation rate coefficients for the collisions of CO2 with helium and neon atoms. *Chemical Physics*, **1982**, 65, 247-257	2.3	45
252	Classical-trajectory calculations on Ar+ sputtering of a Si(001) surface using an ab initio potential. *Physical Review B*, **1989**, 39, 7680-7696	3.3	44
251	Vibrational predissociation of the Ne–C2H4 and Ar–C2H4 van der Waals complexes. *Journal of Chemical Physics*, **1984**, 81, 4474-4480	3.9	44
250	Variational calculations on many-electron diatomic molecules using Hylleraas-type wavefunctions. *Molecular Physics*, **1977**, 34, 793-811	1.7	44
249	Rate Constants for the CH4 + H -> CH3 + H2 Reaction Calculated with a Generalized Reduced-Dimensionality Method. *Journal of Physical Chemistry A*, **2002**, 106, 8256-8260	2.8	43
248	Quantum Simulation of Phenol–Water Clusters. *Journal of Physical Chemistry A*, **2000**, 104, 5590-5599	2.8	43
247	Weakly bound NeHF. *Journal of Chemical Physics*, **1989**, 91, 711-721	3.9	43
246	Isotope and potential energy surface effects in vibrational bonding. *The Journal of Physical Chemistry*, **1984**, 88, 2758-2764		43
245	Kinetic Isotope Effects in the Reactions of D Atoms with CH4, C2H6, and CH3OH: Quantum Dynamics Calculations. *Journal of Physical Chemistry A*, **2004**, 108, 8966-8972	2.8	42
244	A full-dimensional quantum dynamical study of vibrational relaxation in H2+H2. *Chemical Physics Letters*, **2002**, 363, 523-528	2.5	42
243	Reactive scattering of highly vibrationally excited oxygen molecules: Ozone formation?. *Journal of Chemical Physics*, **1998**, 108, 3566-3573	3.9	42

242	Rotationally inelastic and bound state dynamics of H2-OH(X2). *Molecular Physics*, **1994**, 83, 405-428	1.7	40
241	Quantum calculations on the collisions of nonlinear triatomic molecules with atoms: Vibrational excitation in He+SO2(v1v2v3). *Journal of Chemical Physics*, **1981**, 75, 2899-2907	3.9	40
240	The infinite-order-sudden method for light-heavy-light reactions: Application to D+HCl->DCl+H. *Journal of Chemical Physics*, **1982**, 76, 5027-5033	3.9	39
239	Molecules on Ice. *Science*, **1996**, 271, 1509-1509	33.3	38
238	Vibrational predissociation in D2HF. *Journal of Chemical Physics*, **1992**, 96, 90-97	3.9	38
237	An ab Initio Calculation of the Low Rotation-Vibration Energies of the CO Dimer. *Journal of Molecular Spectroscopy*, **1993**, 157, 208-219	1.3	38
236	Coupled states calculations on vibrational relaxation in He+CO2(0110) and He+CO. *Journal of Chemical Physics*, **1987**, 86, 802-812	3.9	38
235	Ab initio calculations on indole-water, 1-methylindole-water and indole-(water)2. *Chemical Physics Letters*, **2000**, 331, 253-261	2.5	37
234	A new method for calculating the rovibrational states of polyatomics with application to water dimer. *Journal of Chemical Physics*, **1995**, 102, 4390-4399	3.9	37
233	A theory for the photodissociation of polyatomic molecules, with application to CF3I. *Journal of Chemical Physics*, **1986**, 84, 4288-4298	3.9	37
232	CI-Hylleraas variational calculation on the ground state of the neon atom. *Physical Review A*, **1976**, 14, 1607-1613	2.6	37
231	Application of the vibrationally adiabatic and static distorted wave born approximation of the reaction H + F2(= 0, j = 0) -> HF(,j?) + F. *Chemical Physics Letters*, **1979**, 66, 493-497	2.5	37
230	Nuclear quantum effects on the structure and energetics of (H2O)6H+. *Physical Chemistry Chemical Physics*, **2005**, 7, 2324-32	3.6	36
229	A Quantum Study on the Reaction between C(3P) and Acetylene. *Journal of Physical Chemistry A*, **2001**, 105, 2694-2707	2.8	36
228	Quantum scattering calculations on the SN2 reaction Cl-CH3Br->ClCH3+Br. *Journal of Chemical Physics*, **1999**, 110, 9483-9491	3.9	35
227	Product CN Rotational Distributions from the H + HCN Reaction. *The Journal of Physical Chemistry*, **1995**, 99, 13664-13669		35
226	Torsional path integral Monte Carlo method for calculating the absolute quantum free energy of large molecules. *Journal of Chemical Physics*, **2003**, 119, 68-76	3.9	34
225	Quantum-mechanical study of the resonances of the SN2 reaction Cl-+CH3Cl->ClCH3+Cl-. *Physical Chemistry Chemical Physics*, **1999**, 1, 1197-1203	3.6	34

224	Rovibrational spectra of open-shell van der Waals complexes: H2□OH (X 2□). *Journal of Chemical Physics*, **1993**, 98, 1843-1855	3.9	34
223	Adsorption of HCL on ice under stratospheric conditions: A computational study. *Geophysical Research Letters*, **1992**, 19, 1355-1358	4.9	34
222	Reduced dimensionality spin-orbit dynamics of CH3 + HCl ? CH4 + Cl on ab initio surfaces. *Journal of Chemical Physics*, **2011**, 134, 204311	3.9	33
221	The effect of the symmetric and asymmetric stretching vibrations of CH4 on the O(3P)+CH4->OH+CH3 reaction. *Physical Chemistry Chemical Physics*, **2000**, 2, 4105-4114	3.6	33
220	Rate constant calculations on the N(4S)+OH(2□) reaction. *Chemical Physics Letters*, **2006**, 431, 261-266	2.5	32
219	Mechanism of photoinduced changes in the structure and optical properties of amorphous As2S3. *Physical Review Letters*, **2000**, 85, 3305-8	7.4	32
218	Rotational and vibrational-rotational relaxation in collisions of CO2(0110) with He atoms. *Journal of Chemical Physics*, **1983**, 78, 4915-4923	3.9	32
217	An improved treatment of spectator mode vibrations in reduced dimensional quantum dynamics: application to the hydrogen abstraction reactions mu + CH4, H + CH4, D + CH4, and CH3 + CH4. *Journal of Chemical Physics*, **2009**, 131, 044111	3.9	31
216	Improving reduced dimensionality quantum reaction dynamics with a generalized transition state. Application to CH4+O(3P). *Journal of Chemical Physics*, **2001**, 115, 2188-2197	3.9	31
215	Potential energy surface effects on differential cross sections for polyatomic reactions. *Chemical Physics*, **1995**, 191, 223-233	2.3	31
214	Calculations on vibrational predissociation of Ar□OH (A 2□). *Journal of Chemical Physics*, **1991**, 95, 8149-8165	3.9	31
213	Rates for the reactions of open-shell ions with molecules. *Chemical Physics Letters*, **1990**, 167, 1-6	2.5	31
212	Low-temperature reactions of He+ and C+ with HCl, SO2 and H2S. *Chemical Physics Letters*, **1988**, 143, 130-134	2.5	31
211	Infrared spectrum of NeHF. *Physical Review Letters*, **1988**, 61, 1576-1579	7.4	31
210	Validity of the rotational sudden approximation for vibrational relaxation in He + CO. *Chemical Physics Letters*, **1983**, 101, 269-273	2.5	31
209	Close-coupling calculations on the H+BrH->HBr+H reaction in three dimensions. *Journal of Chemical Physics*, **1985**, 83, 1685-1692	3.9	31
208	Hylleraas-type wavefunction for lithium hydride. *Chemical Physics Letters*, **1977**, 51, 483-486	2.5	31
207	Collision-induced conformational changes in glycine. *Journal of Chemical Physics*, **2005**, 122, 244323	3.9	30

206	Isotopic branching in (He, HD+) collisions: A time-dependent quantum mechanical study in three dimensions. *Journal of Chemical Physics*, **1999**, 111, 10910-10918	3.9	30
205	Isotopic branching ratio for the O++ HD reaction. *Journal of the Chemical Society, Faraday Transactions 2*, **1989**, 85, 1685		30
204	Quantum and quasiclassical study of the collinear reaction O(3P) + H2 -> OH + H using a LEPS and fitted AB initio potential energy surface. *Chemical Physics Letters*, **1979**, 68, 154-157	2.5	30
203	Torsional diffusion Monte Carlo: A method for quantum simulations of proteins. *Journal of Chemical Physics*, **2001**, 114, 9725-9732	3.9	29
202	Comparison of variational transition state theory and quantum sudden calculations of three-dimensional rate coefficients for the reactions D(H)+BrH -> DBr(HBr)+H. *Journal of Chemical Physics*, **1983**, 78, 777-782	3.9	29
201	The C6H6(H2O)2 complex: Theoretical predictions of the structure, energetics, and tunneling dynamics. *Journal of Chemical Physics*, **1997**, 106, 849-863	3.9	28
200	Isotope Effects in the Formation of Molecular Hydrogen on a Graphite Surface via an Eley–Rideal Mechanism. *Journal of Physical Chemistry A*, **2002**, 106, 8996-9008	2.8	28
199	Torsional path integral Monte Carlo method for the quantum simulation of large molecules. *Journal of Chemical Physics*, **2002**, 116, 8262	3.9	28
198	Diffusion Monte Carlo studies of isotope-substituted water trimers. *Chemical Physics Letters*, **1996**, 263, 680-686	2.5	28
197	Four-center reactions: A quantal model for H4. *Journal of Chemical Physics*, **1996**, 104, 8413-8423	3.9	28
196	New quantum-dynamical approximation for light-heavy-light chemical reactions in three dimensions theory. *Molecular Physics*, **1981**, 44, 1067-1081	1.7	27
195	The vibrationally adiabatic distorted wave method for direct chemical reactions: Application to X+F2(v = 0, j = 0)->XF(v?, j?, mj?)+F(X = Mu, H, D, T). *Journal of Chemical Physics*, **1981**, 75, 3329-3339	3.9	27
194	Calculation of expectation values of molecular systems using diffusion Monte Carlo in conjunction with the finite field method. *Journal of Chemical Physics*, **1994**, 101, 6353-6355	3.9	26
193	A theory for Coriolis enhanced vibrational energy transfer and its application to D2CO + rare gas collisions. *Molecular Physics*, **1986**, 59, 529-545	1.7	26
192	Propensity rules in rotationally inelastic collisions of CO2. *Chemical Physics Letters*, **1983**, 98, 319-323	2.5	26
191	Comparison of the Floquet and rotating-wave methods for multiphoton excitation of sulfur hexafluoride. *The Journal of Physical Chemistry*, **1983**, 87, 735-739		26
190	The O(3 P) + H2(? 2, j, mj) ->OH(? 2, j?, mj?) + H reaction. *Molecular Physics*, **1980**, 41, 689-702	1.7	26
189	An efficient route to thermal rate constants in reduced dimensional quantum scattering simulations: applications to the abstraction of hydrogen from alkanes. *Journal of Chemical Physics*, **2011**, 135, 094311	3.9	25

188	Chemical reaction surface vibrational frequencies evaluated in curvilinear internal coordinates: Application to H + CH(4) H(2) + CH(3). *Journal of Chemical Physics*, **2009**, 130, 024106	3.9	25
187	Vibrational energy transfer in collisions of He atoms with para-difluorobenzene. *Journal of Chemical Physics*, **1987**, 86, 813-821	3.9	25
186	Chemistry as a function of solvation number. Solvated-ion reations in the gas phase and comparison with solution. *Faraday Discussions of the Chemical Society*, **1988**, 85, 37		25
185	CHEMISTRY. Quantum dynamics in the smallest water droplet. *Science*, **2016**, 351, 1267-8	33.3	24
184	Reduced dimensionality quantum dynamics of CH3 + CH4 --> CH4 + CH3: symmetric hydrogen exchange on an Ab initio potential. *Journal of Physical Chemistry A*, **2009**, 113, 4255-64	2.8	24
183	Iterative solution in quantum scattering theory. The log derivative Kohn approach. *Journal of the Chemical Society, Faraday Transactions*, **1990**, 86, 1641		24
182	The significance of fermi resonance for the collisions of triatomic molecules with atoms. *Chemical Physics Letters*, **1980**, 74, 454-458	2.5	24
181	A Simplified Reduced-Dimensionality Study to Treat Reactions of the Type X + CZ3Y -> XY + CZ3□ *Journal of Physical Chemistry A*, **2003**, 107, 10851-10856	2.8	23
180	Excitation of torsional modes of proteins via collisional energy transfer: A quantum dynamical approach. *Journal of Chemical Physics*, **2002**, 116, 9829-9838	3.9	23
179	Quaternion formulation of diffusion quantum Monte Carlo for the rotation of rigid molecules in clusters. *Journal of Chemical Physics*, **2000**, 113, 5193	3.9	23
178	Distorted-wave calculations for the three dimensional chemical reaction H + H2(v ? 2, j = 0) -> H2(v? ? 2, j?, m) + H. *Chemical Physics*, **1980**, 48, 175-181	2.3	23
177	New quantum-dynamical approximation for light-heavy-light chemical reactions in three dimensions. *Molecular Physics*, **1981**, 44, 1083-1097	1.7	23
176	Rate constants of chemical reactions from semiclassical transition state theory in full and one dimension. *Journal of Chemical Physics*, **2016**, 144, 244116	3.9	23
175	Quantum scattering study of the abstraction reactions of H atoms from CH3NH2. *Chemical Physics Letters*, **2007**, 438, 1-7	2.5	22
174	Diffusion Monte Carlo simulations of the dipole-bound state of the water dimer anion. *Journal of Chemical Physics*, **1999**, 111, 10559-10565	3.9	22
173	Reaction rates of ions with dipolar molecules in 2□electronic states. *Journal of Chemical Physics*, **1992**, 96, 1053-1061	3.9	22
172	Prediction of the spectrum for excitation of the van der Waals modes in ArHCN. *Journal of Chemical Physics*, **1990**, 93, 7666-7675	3.9	22
171	Reaction rates of electrons with dipolar molecules. *International Journal of Mass Spectrometry and Ion Processes*, **1987**, 80, 31-49		22

170	Comparison of semiclassical and quantum-mechanical cross sections and rate constants for CO2(0110) + M -> CO2(000O) + M (M = He, Ne). *Chemical Physics Letters*, **1982**, 90, 27-30	2.5	22
169	Reactive resonances in the F + CHD3 reaction--a quantum dynamics study. *Physical Chemistry Chemical Physics*, **2011**, 13, 4340-56	3.6	21
168	Comparative study of cluster- and supercell-approaches for investigating heterogeneous catalysis by electronic structure methods: tunneling in the reaction N + H --> NH on Ru(0001). *Physical Chemistry Chemical Physics*, **2006**, 8, 1437-44	3.6	21
167	Predicting Conformations of Biomolecules: Application to a Noradrenaline Analogue. *Journal of Physical Chemistry B*, **2004**, 108, 2484-2488	3.4	21
166	Quantum mechanical calculations on the Ar++N2 charge transfer reaction. *Journal of Chemical Physics*, **1989**, 90, 1686-1693	3.9	21
165	Quantal sudden calculations on the exchange reactions of vibrationally excited HBr (v = 1) with H and D atoms in three dimensions. *Chemical Physics*, **1983**, 81, 379-391	2.3	21
164	Reduced-Dimensionality Semiclassical Transition State Theory: Application to Hydrogen Atom Abstraction and Exchange Reactions of Hydrocarbons. *Journal of Physical Chemistry A*, **2015**, 119, 12015-27	2.8	20
163	A Combined Theoretical and Experimental Study of Sarin (GB) Decomposition at High Temperatures. *Journal of Physical Chemistry A*, **2017**, 121, 6200-6210	2.8	20
162	Towards understanding a mechanism for reversible hydrogen storage: theoretical study of transition metal catalysed dehydrogenation of sodium alanate. *Physical Chemistry Chemical Physics*, **2010**, 12, 4012-23	3.6	20
161	The effect of the symmetric and asymmetric stretching vibrations on the CH3D+O(3P)->CH3+OD reaction. *Chemical Physics Letters*, **2002**, 363, 529-533	2.5	20
160	The effect of the torsional and stretching vibrations of C2H6 on the H + C2H6 --> H2 + C2H5 reaction. *Journal of Chemical Physics*, **2005**, 123, 64305	3.9	20
159	A quenching method in quantum-classical studies of dynamics with a bifurcating wavefunction. *Chemical Physics Letters*, **1996**, 262, 284-291	2.5	20
158	Calculations on the van der Waals spectrum of Ar-Tetrazine. *Journal of Chemical Physics*, **1990**, 92, 5875-5884	3.9	20
157	Rotationally and vibrationally inelastic scattering of glyoxal at E=80 meV. *Journal of Chemical Physics*, **1990**, 93, 287-311	3.9	20
156	Coupled channel calculations on the vibrational predissociation of the ethylene dimer. *Chemical Physics Letters*, **1986**, 125, 477-480	2.5	20
155	Decoupling the vibrational modes in triatomic molecule collision calculations. *Molecular Physics*, **1981**, 43, 469-481	1.7	20
154	An investigation of one- versus two-dimensional semiclassical transition state theory for H atom abstraction and exchange reactions. *Journal of Chemical Physics*, **2016**, 144, 084113	3.9	20
153	New Developments in Semiclassical Transition-State Theory. *Journal of Physical Chemistry A*, **2019**, 123, 4639-4657	2.8	19

152	Speed improvement of diffusion quantum Monte Carlo calculations on weakly bound clusters. *Chemical Physics Letters*, **1998**, 283, 269-276	2.5	19
151	Torsional anharmonicity in transition state theory calculations. *Physical Chemistry Chemical Physics*, **2007**, 9, 2397-405	3.6	19
150	Surface Coverage Effects on the Formation of Molecular Hydrogen on a Graphite Surface via an Eley□Rideal Mechanism. *Journal of Physical Chemistry A*, **2003**, 107, 10862-10871	2.8	19
149	Diffusion Monte Carlo simulations on uracil□water using an anisotropic atom□atom potential model. *Faraday Discussions*, **2001**, 118, 95-108	3.6	19
148	Diffusion Monte Carlo simulations of methanol□water clusters. *Chemical Physics Letters*, **1999**, 301, 275-280	2.5	19
147	Reactions of strongly polar ions with molecules. *Chemical Physics Letters*, **1995**, 232, 267-272	2.5	19
146	Reactions of O(3P) with saturated hydrocarbons: Vibrationally adiabatic distorted wave calculations of product rotational distributions for two triatomic model reactions. *Journal of Chemical Physics*, **1986**, 84, 2620-2623	3.9	19
145	Quantum-dynamical study of the translational-vibrational energy transfer in the collinear collisions of atoms with triatomic molecules. *Molecular Physics*, **1980**, 39, 1295-1310	1.7	19
144	Exchange reactions of hydrogen halides with hydrogenic atoms. *Chemical Physics*, **1982**, 71, 117-125	2.3	19
143	Chemistry. Quantum chemistry of complex systems. *Science*, **2006**, 314, 265-6	33.3	18
142	Torsional anharmonicity in the conformational thermodynamics of flexible molecules. *Molecular Physics*, **2005**, 103, 1573-1578	1.7	18
141	Quantum initial value representation simulation of water trimer far infrared absorption spectrum. *Journal of Chemical Physics*, **2004**, 120, 5608-15	3.9	18
140	The importance of tunneling in the first hydrogenation step in ammonia synthesis over a Ru(0001) surface. *Journal of Chemical Physics*, **2005**, 122, 134702	3.9	18
139	A comparison of the vibrational predissociation rates in the rare-gas□ethylene clusters. *Journal of the Chemical Society, Faraday Transactions 2*, **1987**, 83, 1719-1731		18
138	Test of a modified sudden approximation for rotational excitation in He + CH3CN. *Chemical Physics*, **1987**, 112, 15-22	2.3	18
137	Vibrationally adiabatic distorted wave calculation for the rotationally excited reaction H+H2(v = 0, j)->H2(v? = 0, j?)+H. *Journal of Chemical Physics*, **1981**, 74, 6991-6993	3.9	18
136	Computational molecular spectroscopy. *Nature Reviews Methods Primers*, **2021**, 1,		18
135	Quantum dynamics study of the Langmuir□Hinshelwood H+H recombination mechanism and H2 formation on a graphene model surface. *Chemical Physics*, **2007**, 338, 1-10	2.3	17

134	Observational Indicators of Formation Excitation of H2. *Astrophysics and Space Science*, **2003**, 288, 377-389	1.6	17
133	H2 dissociation on metal surfaces: Six-dimensional approximate quantum calculations. *Journal of Chemical Physics*, **1996**, 105, 5258-5264	3.9	17
132	Rate constant calculations for ion symmetric top and ion asymmetric top reactions. *Journal of the Chemical Society, Faraday Transactions*, **1992**, 88, 901-908		17
131	Vibrational predissociation of ArH2O. *Journal of Chemical Physics*, **1992**, 97, 8111-8122	3.9	17
130	Competition between vibrational and rotational excitation in glyoxal. *Chemical Physics Letters*, **1989** , 154, 62-66	2.5	17
129	Van der waals bound states and intermolecular bend-stretch coupling in Ne?C2H4 and Ar-tetrazine. *Chemical Physics*, **1989**, 139, 67-88	2.3	17
128	Effect of rotational excitation on chemical reaction cross sections. *Molecular Physics*, **1983**, 48, 619-629	1.7	17
127	Proton transfer as a function of hydration number and temperature: rate constants and product distributions for OH-(H2O)0,1,2,3 + HF at 200-500 K. *Journal of the American Chemical Society*, **1986**, 108, 3140-3142	16.4	17
126	Comparison of the rotationally adiabatic and vibrationally adiabatic distorted wave methods for the H + H2(v=0, j=0)->H2(v?=0,j?)+H and D + H2(v=0, j=0)->DH(v?=0, j?)+H chemical reactions. *Molecular Physics*, **1981**, 43, 621-639	1.7	17
125	Vibrational excitation of SF6 in collisions with He atoms. *Chemical Physics*, **1982**, 64, 413-419	2.3	17
124	Quantum effects in the abstraction reaction by H atoms of primary and secondary hydrogens in n-C4H10: a test of a new potential energy surface construction method. *Physical Chemistry Chemical Physics*, **2013**, 15, 1222-31	3.6	16
123	Quantum dynamics and kinetics of the abstraction reactions by H atoms of primary and secondary hydrogens in C3H8. *Molecular Physics*, **2005**, 103, 1745-1755	1.7	16
122	Calculation of the energy levels of weakly bound molecular trimers: Application to (H2)3. *Journal of Chemical Physics*, **2002**, 117, 7512-7519	3.9	16
121	Quantum simulation of weakly bound complexes using direct ab initio energy points. *Chemical Physics Letters*, **1995**, 237, 39-44	2.5	16
120	Quantum-mechanical calculations of collinear atom-triatom transition probabilities for anharmonic triatom potentials. *Chemical Physics Letters*, **1980**, 72, 264-268	2.5	16
119	Quantum dynamical examination of surprisal theory for the three-dimensional hydrogen exchange reaction. *Chemical Physics Letters*, **1978**, 59, 437-442	2.5	16
118	Fast reactions between diatomic and polyatomic molecules. *The Journal of Physical Chemistry*, **1992**, 96, 7346-7351		15
117	Electronic spectrum of the Ar?OH complex: effect of isotopic substitution and temperature. *Chemical Physics Letters*, **1990**, 173, 541-550	2.5	15

116	Calculations on Ar+ sputtering of a Cu surface using an ab initio potential. *Surface Science*, **1988**, 202, 320-334	1.8	15
115	Collisions of polyatomic molecules with solid surfaces: A semiclassical stochastic trajectory approach. *Journal of Chemical Physics*, **1984**, 81, 5167-5178	3.9	15
114	Torsional anharmonicity in the conformational analysis of tryptamine. *Physical Chemistry Chemical Physics*, **2007**, 9, 2065-74	3.6	14
113	Chemistry. Geometric phase in chemical reactions. *Science*, **2005**, 309, 1195-6	33.3	14
112	Reaction path zero-point energy from diffusion Monte Carlo calculations. *Journal of Chemical Physics*, **1995**, 102, 1592-1596	3.9	14
111	Experimental and theoretical determination of rate constants for vibrational relaxation of CO2 and CH3F by He. *Chemical Physics*, **1987**, 117, 9-16	2.3	14
110	Vibrational energy transfer in organic molecules. 1. Helium + cyclopropane. *Journal of the American Chemical Society*, **1984**, 106, 970-975	16.4	14
109	Vibrational predissociation of the ethylene dimer. *Faraday Discussions of the Chemical Society*, **1986**, 82, 327		14
108	Application of a dynamical S matrix method to the three-dimensional H+H2 exchange reaction. *Journal of Chemical Physics*, **1979**, 71, 1101-1109	3.9	14
107	Rate coefficient calculations on the three-dimensional D + HCl -> DCl + H reaction using a new quantum-dynamical approximation. *Chemical Physics Letters*, **1981**, 80, 271-274	2.5	14
106	Reaction rates of all hydrogenation steps in ammonia synthesis over a Ru(0001) surface. *Journal of Catalysis*, **2006**, 244, 199-207	7.3	13
105	Quantum dynamics calculations of the Mu + CH4 -> MuH + CH3 reaction rate constants. *Chemical Physics Letters*, **2006**, 421, 499-503	2.5	13
104	Theoretical Investigation of the Surface Reaction N(ads) + H(ads) -> NH(ads) on Ru(0001) Using Density Functional Calculations, Variational Transition-State Theory, and Semiclassical Tunneling Method. *Journal of Physical Chemistry B*, **2004**, 108, 336-345	3.4	13
103	Photodissociation of carbon dioxide and reactive scattering resonances. *The Journal of Physical Chemistry*, **1987**, 91, 1580-1584		13
102	Quantum dynamics of the abstraction reaction of H with cyclopropane. *Journal of Physical Chemistry A*, **2014**, 118, 10134-43	2.8	12
101	Calculation of the vibrational spectral density of NO2 via density correlation functions. *Chemical Physics Letters*, **1997**, 273, 55-61	2.5	12
100	Quantum simulation of a hydrated noradrenaline analog with the torsional path integral method. *Journal of Physical Chemistry A*, **2006**, 110, 731-40	2.8	12
99	Microscopic mechanisms for photoinduced metastability in amorphous As2S3. *Physical Review B*, **2002**, 65,	3.3	12

98	Quantum stereodynamics of four-atom reactions: theory and application to H2+OH<->H2O+H. *Faraday Discussions*, **1999**, 113, 119-132	3.6	12
97	Electronic spectra of the OH(A2Π)-H2 and OH(A2Π)-D2 complexes. *Chemical Physics Letters*, **1995**, 244, 421-426	2.5	12
96	Coupled channel calculations on the vibrational predissociation of argon-para-difluorobenzene. *Chemical Physics*, **1989**, 129, 125-147	2.3	12
95	Semiclassical calculation of energy transfer in polyatomic molecules. IX. Cross sections for M + CO2 (000) -> M + CO2(nml) (M = He and Ar). *Chemical Physics*, **1983**, 80, 213-219	2.3	12
94	Tunnelling and the kinetic isotope effect in CH3+CH4->CH4+CH3: An application of semiclassical transition state theory. *Chemical Physics Letters*, **2018**, 693, 88-94	2.5	11
93	Calculation of the photodetachment spectrum for H3O-. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 747-753		11
92	Vibrational relaxation in H2+H2: full-dimensional quantum dynamical study. *International Journal of Mass Spectrometry*, **2003**, 223-224, 335-342	1.9	11
91	Vibrational predissociation of D2HF and H2HF with a new potential energy surface. *Molecular Physics*, **1998**, 93, 619-625	1.7	11
90	Vibrational relaxation in NO+?He: accurate quantum mechanical study. *International Journal of Mass Spectrometry and Ion Processes*, **1995**, 149-150, 207-215		11
89	Rate coefficient expressions for reactions of molecules in 2Σ electronic states at low temperatures. *Journal of Chemical Physics*, **1993**, 98, 420-426	3.9	11
88	Infinite order sudden calculation of Raman Q-branch linewidths for H2O+H2O. *Journal of Chemical Physics*, **1991**, 95, 1037-1048	3.9	11
87	Vibrational energy transfer in organic molecules. *Molecular Physics*, **1984**, 51, 1299-1310	1.7	11
86	Validity of the breathing sphere method for atom-triatomic molecule collisions. *Chemical Physics Letters*, **1981**, 81, 21-25	2.5	11
85	Torsional anharmonicity in the conformational analysis of beta-D-galactose. *Journal of Physical Chemistry B*, **2006**, 110, 3485-92	3.4	10
84	Coupled states calculations on vibrational relaxation of N+2 in collisions with He. *Chemical Physics Letters*, **1994**, 219, 366-371	2.5	10
83	Rotationally inelastic rates and Raman Q-branch linewidths for N2 + N2. *Molecular Physics*, **1991**, 73, 317-333	1.7	10
82	Vibrationally induced photodetachment of electrons from negative molecular ions. *Physical Review A*, **1989**, 40, 4392-4399	2.6	10
81	Reactions of nitrogen(1+) and hydrogen trimer (1+) with the structural isomers of dichloroethene. *The Journal of Physical Chemistry*, **1988**, 92, 6572-6574		10

80	Method for the determination of parametric potential energy surfaces by the direct inversion of inelastic scattering data. *Journal of Chemical Physics*, **1985**, 83, 4470-4475	3.9	10
79	Catalysis and tunnelling in the unimolecular decay of Criegee intermediates. *Physical Chemistry Chemical Physics*, **2018**, 20, 25224-25234	3.6	10
78	Crossed-beam and reduced dimensionality studies of the state-to-state integral cross sections of the Cl+HCD3(v)->HCl(v?)+CD3 reaction. *Chemical Physics Letters*, **2013**, 587, 88-92	2.5	9
77	Quantum study on the branching ratio of the reaction NO2+OH. *Journal of Chemical Physics*, **2007**, 126, 154321	3.9	9
76	Prediction of the infrared spectrum for the neon□ethylene van der Waals complex. *Journal of Chemical Physics*, **1989**, 91, 1079-1091	3.9	9
75	Rotationally and vibrationally inelastic scattering of glyoxal by helium at an energy of 96 meV. *Chemical Physics*, **1990**, 148, 359-379	2.3	9
74	New type of rotational basis function for quantum-mechanical molecular collision calculations. *Chemical Physics*, **1983**, 76, 331-341	2.3	9
73	Glory undulations in total integral collision cross sections. *Molecular Physics*, **1983**, 49, 1139-1147	1.7	9
72	Approximate calculation of vibrationally inelastic molecular collision cross sections. *Chemical Physics Letters*, **1985**, 114, 205-209	2.5	9
71	Quantum dynamical study of molecular overtone transitions induced by intense laser radiation. *Molecular Physics*, **1982**, 46, 1099-1108	1.7	9
70	Ionization potentials of cycloalkenes. *Journal of the Chemical Society, Faraday Transactions 2*, **1974**, 70, 1889		9
69	A method to calculate vibrational frequency shifts in heteroclusters: application to N2+□len. *Journal of the Chemical Society, Faraday Transactions*, **1996**, 92, 11-15		8
68	Theoretical study of ion assisted chemical reactions on a semiconductor solid. Model: Ar++Cl2/Si(001). *Journal of Applied Physics*, **1986**, 60, 1183-1188	2.5	8
67	Fourier transform method for the classical trajectory problem. *Journal of Chemical Physics*, **1979**, 71, 1372-1379	3.9	8
66	Theoretical Study of Gas-Phase Unimolecular Decomposition of Simulants of the Nerve Agent VX. *Journal of Physical Chemistry A*, **2019**, 123, 59-72	2.8	8
65	Analytic Route to Tunneling Splittings Using Semiclassical Perturbation Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 3486-3493	6.4	7
64	Application of one-dimensional semiclassical transition state theory to the CHOH + H ? CHOH/CHO + H reactions. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2018**, 376,	3	7
63	A reduced dimensionality quantum mechanical study of the H + HCF3 <-> H2 + CF3 reaction. *Physical Chemistry Chemical Physics*, **2013**, 15, 18530-8	3.6	7

62	Classical and approximate quantum investigations of vibrational energy transfer in S1 p-difluorobenzene. *Journal of Chemical Physics*, **1997**, 106, 5439-5453	3.9	7
61	QuasiclassicaltrajectorystudyofthereactionH2+OH->H2O+H: Comparison withquantum results. *Journal of the Chemical Society, Faraday Transactions*, **1997**, 93, 841-846		7
60	The vibrational predissociation of HeBr2: a wavepacket study. *Chemical Physics Letters*, **1997**, 271, 171-177	2.5	7
59	Time-resolved dissociation of the H2OH entrance channel complex. *Chemical Physics Letters*, **1998**, 294, 518-522	2.5	7
58	Fast reactions between a linear molecule and a polar symmetric top. *Computational and Theoretical Chemistry*, **1995**, 341, 53-61		7
57	Classical trajectory calculations of non-linear sputtering: SiCl4 sputtering of a Cu(001) surface using ab initio potentials. *Surface Science*, **1990**, 227, 369-389	1.8	7
56	Sputtering of a Cu solid by SiCl4molecules. *Journal Physics D: Applied Physics*, **1987**, 20, 880-888	3	7
55	Application of scaling theory to vibrational relaxation in linear anharmonic triatomic molecules. *Journal of Chemical Physics*, **1983**, 79, 2206-2211	3.9	7
54	The vibrational relaxation of ozone by helium atoms. *Chemical Physics Letters*, **1982**, 87, 407-411	2.5	7
53	Subsurface effects in the dissociation of H2 on Pd(111). *Chemical Physics Letters*, **1997**, 266, 437-442	2.5	6
52	Rates of the reaction C2 H3 +H2 ->C2H4+H. *Molecular Physics*, **2006**, 104, 151-158	1.7	6
51	A noninvasive rf probe for the study of ionization and dissociation processes in technological plasmas. *Journal of Applied Physics*, **1999**, 86, 4100-4106	2.5	6
50	Reduced-dimension quantum calculations for molecule-surface reactions. *Chemical Physics Letters*, **1995**, 246, 399-404	2.5	6
49	Potential energy functions of polyatomic molecules. *Chemical Physics*, **1979**, 41, 387-394	2.3	6
48	Vibrational energy transfer in diatom-triatom collisions. *Molecular Physics*, **1981**, 42, 1121-1136	1.7	6
47	Photodissociation and reactive scattering resonances. *The Journal of Physical Chemistry*, **1982**, 86, 2569-2571		6
46	Calculations of rate constants for reactions of first and second row cations. *Theoretical Chemistry Accounts*, **1997**, 98, 33-41	1.9	5
45	STIMULATED EMISSION PUMPING AS A PROBE OF THE OH (X2) + Ar INTERMOLECULAR POTENTIAL ENERGY SURFACE. *Advanced Series in Physical Chemistry*, **1995**, 659-688		5

44	Resonance enhancement of vibrational relaxation of glyoxal in collisions with helium at low temperatures. *Chemical Physics*, **1990**, 140, 255-263	2.3	5
43	Distorted wave calculations of vibrational excitation in CO2+He and CO2+Ar collisions. *Chemical Physics*, **1987**, 114, 221-229	2.3	5
42	Quantum test of quasiclassical calculations on atom triatom collisions. *Journal of Chemical Physics*, **1981**, 75, 2023-2025	3.9	5
41	Spiers Memorial Lecture. Introductory lecture: quantum dynamics of chemical reactions. *Faraday Discussions*, **2018**, 212, 9-32	3.6	4
40	Quantum mechanical study of the vibrational relaxation of O2+ colliding with Kr. *Journal of Chemical Physics*, **1999**, 111, 1972-1978	3.9	4
39	Mode-selective decay dynamics of the ortho-H2 OH complex: experiment and theory. *Molecular Physics*, **1999**, 97, 151-158	1.7	4
38	The influence of collisions on laser absorption spectra of SF6. *Chemical Physics*, **1989**, 135, 91-97	2.3	4
37	Triatom-triatom collisions: Fixed angle close-coupling study of vibrational excitation in the 12CO2+13CO2 system. *Chemical Physics*, **1981**, 57, 297-309	2.3	4
36	Diffusion Monte Carlo studies of water clusters. *Advances in Molecular Vibrations and Collision Dynamics*, **1998**, 311-363		4
35	Molecules in confinement in clusters, quantum solvents and matrices: general discussion. *Faraday Discussions*, **2018**, 212, 569-601	3.6	4
34	Time-dependent wavepacket calculations on polyatomic reactive scattering. *Computer Physics Communications*, **1998**, 108, 191-199	4.2	3
33	The thermodesorption mechanism of ammonia from Ru(0 0 0 1). *Surface Science*, **2006**, 600, 1054-1059	1.8	3
32	Tunnelling in cyclocarbenes: An application of Semiclassical Transition State Theory in reduced dimensions. *Chemical Physics Letters*, **2019**, 735, 136783	2.5	2
31	Quasiclassical trajectory calculations of hydrogen absorption in the (NaAlH4)2Ti system on a model analytical potential energy surface. *Physical Chemistry Chemical Physics*, **2012**, 14, 3915-21	3.6	2
30	Femtochemistry and femtobiology. *Chemical Physics*, **2008**, 350, 1	2.3	2
29	Non-orthogonal basis sets for hyperspherical coordinate calculations on chemical reactions. *Chemical Physics Letters*, **2001**, 346, 149-154	2.5	2
28	CHEMICAL PHYSICS:Interfering with Water. *Science*, **1999**, 285, 1218-1219	33.3	2
27	Coupled channel calculations on rovibrational excitation of H2O in collisions with H atoms. *Chemical Physics*, **1993**, 175, 23-36	2.3	2

26	Ion-dipole fragmentations. *Molecular Physics*, **1989**, 67, 1099-1115	1.7	2
25	Laser-induced isomerization of trimethylenimine. *The Journal of Physical Chemistry*, **1983**, 87, 3025-3027		2
24	Use of localized rotational basis functions in non-reactive scattering with application to H + HF (v=1 -> 0). *Molecular Physics*, **1984**, 51, 1311-1319	1.7	2
23	Calculations on the unimolecular decomposition of the nerve agent VX. *Physical Chemistry Chemical Physics*, **2020**, 22, 564-574	3.6	2
22	Hydrogen tunnelling in the rearrangements of carbenes: the role of dynamical calculations. *Physical Chemistry Chemical Physics*, **2020**, 22, 962-965	3.6	2
21	Fundamentals: general discussion. *Faraday Discussions*, **2016**, 195, 139-169	3.6	2
20	Quantum Scattering and Semiclassical Transition State Theory Calculations on Chemical Reactions of Polyatomic Molecules in Reduced Dimensions. *Advances in Chemical Physics*, **2018**, 117-149		1
19	Chemistry. 100 years of atomic theory. *Science*, **2013**, 341, 244-5	33.3	1
18	Computational studies of protein–peptide interactions with systematic mutation of residues. *Molecular Physics*, **2004**, 102, 939-951	1.7	1
17	Vibrationally inelastic collision cross sections of He+SO2: Distorted wave approach. *Journal of Chemical Physics*, **1989**, 91, 3509-3515	3.9	1
16	Summing the partial-wave series in molecular collision calculations. *Computer Physics Communications*, **1988**, 48, 223-228	4.2	1
15	Chemical Reactions **2002**, 1068-1080		1
14	Predictions of Spectra for Van der Waals Molecules. *NATO ASI Series Series B: Physics*, **1990**, 355-369		1
13	John Norman Murrell. 2 March 1932 – 25 January 2016. *Biographical Memoirs of Fellows of the Royal Society*, **2017**, 63, 467-486	0.1	0
12	Historical perspective on: Semiclassical trajectory approach to photoisomerisation by A Warshel and M. Karplus [Chem. Phys. Lett. 32 (1) (1975) 11–17]. *Chemical Physics Letters*, **2013**, 589, 67	2.5	
11	Perspective on "Quantum mechanical reactive scattering for three-dimensional atom plus diatom systems. II. Accurate cross sections for H + H2". *Theoretical Chemistry Accounts*, **2000**, 103, 326-327	1.9	
10	Calculation of product branching ratios for the reaction of an ion with a molecule in a 2-electronic state. *Chemical Physics*, **1994**, 185, 57-63	2.3	
9	Rotationally and vibrationally inelastic scattering of 41 D2CO. *Chemical Physics*, **1992**, 163, 339-349	2.3	

List of Publications

8	Computational analyses of the vibrational spectra of fentanyl, carfentanil and remifentanil.. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 270, 120763	4.4
7	Simulation of Water Clusters with Rigid-Body Diffusion Monte Carlo **2000**, 187-199	
6	Perspective on Quantum mechanical reactive scattering for three-dimensional atom plus diatom systems. II. Accurate cross sections for H + H2 **2000**, 326-327	
5	A Quantum Model Hamiltonian to Study X + YCZ3 <-> XY + CZ3 Reactions. *Lecture Notes in Quantum Chemistry II*, **2000**, 286-290	0.6
4	Quantum Dynamics of Gas-Phase SN2 Reactions. *Lecture Notes in Quantum Chemistry II*, **2000**, 299-302	0.6
3	Temperature-Dependent Rate Constants for Ion-Dipole Reactions: C+(2P) + HCl(X 1) **1989**, 327-338	
2	Quantum dynamics of isolated molecules: general discussion. *Faraday Discussions*, **2018**, 212, 281-306	3.6
1	Amyand David Buckingham. 28 January 1930 4 February 2021. *Biographical Memoirs of Fellows of the Royal Society*, **2022**, 72, 77-99	0.1