David C Clary

List of Publications by Year
in descending order

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356 papers	17,259 citations	17405 63 h-index	20900 115 g-index
376 all docs	376 docs citations	376 times ranked	8009 citing authors

#	Article	IF	Citations
1	Definition of the hydrogen bond (IUPAC Recommendations 2011). Pure and Applied Chemistry, 2011, 83, 1637-1641.	0.9	1,449
2	Defining the hydrogen bond: An account (IUPAC Technical Report). Pure and Applied Chemistry, 2011, 83, 1619-1636.	0.9	856
3	The Water Dipole Moment in Water Clusters. Science, 1997, 275, 814-817.	6.0	635
4	Characterization of a cage form of the water hexamer. Nature, 1996, 381, 501-503.	13.7	624
5	Potential optimized discrete variable representation. Chemical Physics Letters, 1992, 190, 225-230.	1.2	567
6	QUANTUMSCATTERINGCALCULATIONS ONCHEMICALREACTIONS. Annual Review of Physical Chemistry, 2003, 54, 493-529.	4.8	371
7	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.	2.9	245
8	Fast Chemical Reactions: Theory Challenges Experiment. Annual Review of Physical Chemistry, 1990, 41, 61-90.	4.8	214
9	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	1.2	192
10	Rates of chemical reactions dominated by long-range intermolecular forces. Molecular Physics, 1984, 53, 3-21.	0.8	191
11	Quantum reactive scattering of fourâ€atom reactions with nonlinear geometry: OH+H2â†'H2O+H. Journal of Chemical Physics, 1991, 95, 7298-7310.	1.2	190
12	Four-Atom Reaction Dynamics. The Journal of Physical Chemistry, 1994, 98, 10678-10688.	2.9	163
13	Calculations of rate constants for ion-molecule reactions using a combined capture and centrifugal sudden approximation. Molecular Physics, 1985, 54, 605-618.	0.8	157
14	Quantum Theory of Chemical Reaction Dynamics. Science, 1998, 279, 1879-1882.	6.0	149
15	Calculations of the tunneling splittings in water dimer and trimer using diffusion Monte Carlo. Journal of Chemical Physics, 1995, 102, 7817-7829.	1.2	144
16	Sticking of hydrogen chloride and chlorine hydroxide to ice: a computational study. The Journal of Physical Chemistry, 1992, 96, 7079-7088.	2.9	143
17	Combiningabinitiocomputations, neural networks, and diffusion Monte Carlo: An efficient method to treat weakly bound molecules. Journal of Chemical Physics, 1996, 105, 7597-7604.	1.2	135
18	Interaction of HCl with water clusters: (H2O)nHCl, n = 1-3. The Journal of Physical Chemistry, 1995, 99, 14323-14333.	2.9	127

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19	Ab Initio Calculations on Uracilâ˜Water. Journal of Physical Chemistry A, 1999, 103, 1611-1618.	1.1	119
20	Application of hyperspherical coordinates to fourâ€atom reactive scattering: H2+CNâ†'H+HCN. Journal of Chemical Physics, 1990, 92, 4178-4190.	1.2	118
21	Quantum scattering calculations on the OH+H2(v=0,1), OH+D2, and OD+H2reactions. Journal of Chemical Physics, 1992, 96, 3656-3665.	1.2	118
22	The dynamics of the reaction OH + D2 â†' HOD + D: Crossed beam experiments and quantum mechanical scattering calculations on ab initio potential energy surfaces. Chemical Physics, 1996, 207, 389-409.	0.9	114
23	A quantum model Hamiltonian to treat reactions of the type X+YCZ3â†'XY+CZ3: Application to O(3P)+CH4â†'OH+CH3. Journal of Chemical Physics, 2000, 112, 1859-1867.	1.2	112
24	Quantum and quasiclassical calculations on the OH+COâ†'CO2+H reaction. Journal of Chemical Physics, 1993, 99, 4578-4589.	1.2	108
25	Temperature dependence of rate coefficients for reactions of ions with dipolar molecules. Chemical Physics Letters, 1985, 119, 320-326.	1.2	106
26	Quantum dynamical stereochemistry of atomâ€"diatom reactions. Journal of Chemical Physics, 1997, 106, 4509-4521.	1.2	105
27	Interstellar carbon chemistry: Reaction rates of neutral atomic carbon with organic molecules. Astrophysical Journal, 1994, 422, 416.	1.6	102
28	Threeâ€body effects on molecular properties in the water trimer. Journal of Chemical Physics, 1995, 103, 8924-8930.	1.2	100
29	Quantum theory of planar fourâ€atom reactions. Journal of Chemical Physics, 1994, 100, 402-422.	1.2	99
30	Mechanisms for supercollisions. Faraday Discussions, 1995, 102, 423.	1.6	99
31	New Potential Energy Function for Four-Atom Reactions. Application to OH + H2. Journal of Physical Chemistry A, 1998, 102, 9631-9637.	1.1	98
32	Formation of molecular hydrogen on a graphite surface via an Eleyâ€"Rideal mechanism. Chemical Physics Letters, 2000, 319, 303-308.	1.2	97
33	Mode selective chemistry in the reactions of OH with HBr and HCl. Journal of Chemical Physics, 1994, 101, 3704-3714.	1.2	95
34	Rydbergâ€"Kleinâ€"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.	1.2	94
35	Using quantum rotational polarization moments to describe the stereodynamics of the H+D2(v=0,j=0)â†'HD(vâ€²,jâ€²)+D reaction. Journal of Chemical Physics, 1998, 108, 3142-3153.	1.2	94
36	Quantum theory of four-atom reactions using arrangement channel hyperspherical coordinates: Formulation and application to OH+H2â†"H2O+H. Journal of Chemical Physics, 1997, 107, 8975-8984.	1.2	93

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37	Quantum calculations on the rate constant for the O + OH reaction. Chemical Physics Letters, 1984, 112, 346-350.	1.2	92
38	Photodetachment of electrons from dipolar anions. The Journal of Physical Chemistry, 1988, 92, 3173-3181.	2.9	92
39	Quantum dynamics of the Walden inversion reaction Clâ^'+CH3Clâ†'ClCH3+Clâ^'. Journal of Chemical Physics, 1997, 106, 575-583.	1.2	92
40	Ab initio and diffusion Monte Carlo study of uracilâ€"water, thymineâ€"water, cytosineâ€"water, and cytosineâ€"(water)2. Physical Chemistry Chemical Physics, 2000, 2, 1281-1290.	1.3	88
41	Quantum study of vibrational excitation in the threeâ€dimensional collisions of CO2 with rare gas atoms. Journal of Chemical Physics, 1981, 75, 209-219.	1.2	86
42	Quantum scattering and quasi-classical trajectory calculations for the H2+OH â‡Œ H2O+H reaction on a new potential surface. Physical Chemistry Chemical Physics, 2000, 2, 693-700.	1.3	86
43	Tunneling dynamics in water tetramer and pentamer. Journal of Chemical Physics, 1996, 105, 6626-6633.	1.2	85
44	Time-Dependent Quantum Mechanical Calculations on the Formation of Molecular Hydrogen on a Graphite Surface via an Eleyâ^'Rideal Mechanismâ€. Journal of Physical Chemistry A, 2001, 105, 2173-2182.	1.1	84
45	Calculation of the electronic spectrum for Arâ€"OH. Journal of Chemical Physics, 1990, 93, 3367-3378.	1.2	79
46	C + C2H2: A Key Reaction in Interstellar Chemistry. Journal of Physical Chemistry A, 2002, 106, 5541-5552.	1.1	78
47	Calculation of the intermolecular bound states for water dimer. Journal of Chemical Physics, 1994, 101, 3603-3609.	1.2	77
48	Bond-selected reaction of HOD with H atoms. Chemical Physics Letters, 1992, 192, 34-40.	1.2	76
49	Quantum scattering calculations on the CH4+OHâ†'CH3+H2O reaction. Journal of Chemical Physics, 1994, 101, 5756-5771.	1.2	76
50	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.	1.2	74
51	Computational molecular spectroscopy. Nature Reviews Methods Primers, 2021, 1, .	11.8	73
52	Recent advances in quantum scattering calculations on polyatomic bimolecular reactions. Chemical Society Reviews, 2017, 46, 7625-7649.	18.7	72
53	Chemical reactions dominated by long-range intermolecular forces. Faraday Discussions of the Chemical Society, 1987, 84, 333.	2.2	71
54	Rate constant calculations on fast diatomâ€"diatom reactions. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 1667-1679.	1.7	71

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55	Rate constants for the reactions of ions with dipolar polyatomic molecules. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 139.	1.1	70
56	Slit jet infrared spectroscopy of NeHF complexes: Internal rotor andJâ€dependent predissociation dynamics. Journal of Chemical Physics, 1989, 91, 722-731.	1.2	70
57	Quantum scattering calculations on H2O+Hâ†'H2+OH and isotopes: Rotational distributions and cross sections. Journal of Chemical Physics, 1993, 99, 7774-7786.	1.2	70
58	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.	6.6	69
59	Calculation of van der Waals spectra for H2HF, D2HF, and H2DF. Journal of Chemical Physics, 1990, 93, 6334-6349.	1.2	69
60	Stateâ€selected vibrational relaxation rates for highly vibrationally excited oxygen molecules. Journal of Chemical Physics, 1995, 102, 9544-9556.	1.2	68
61	Calculation of vibrationâ€“rotation spectra for rare gasâ€“HCl complexes. Journal of Chemical Physics, 1989, 90, 7000-7013.	1.2	66
62	Ultraâ€low temperature kinetics of neutralâ€“neutral reactions: New experimental and theoretical results for OH+HBr between 295 and 23 K. Journal of Chemical Physics, 1994, 101, 1748-1751.	1.2	66
63	Quantum dynamics of the O(3P)+CH4â†'CH3+OH reaction. Physical Chemistry Chemical Physics, 1999, 1, 1173-1179.	1.3	66
64	A multifaceted approach to hydrogen storage. Physical Chemistry Chemical Physics, 2011, 13, 16955.	1.3	64
65	Rate coefficients of the reactions of ions with polar molecules at interstellar temperatures. Astrophysical Journal, 1985, 296, L31.	1.6	64
66	Stimulated emission pumping of van der Waals vibrations in the ground electronic state of OHî—¸Ar. Chemical Physics Letters, 1991, 178, 301-310.	1.2	63
67	A study of HOCO resonances in the OH+COâ†'CO2+H reaction. Journal of Chemical Physics, 1994, 101, 2779-2784.	1.2	63
68	Temperature dependence of the rate constant for the Clâ^'+CH3Br reaction down to 23 K. Journal of Chemical Physics, 1997, 107, 1021-1024.	1.2	63
69	Influence of surface defects on the adsorption of HCl on ice. Journal of the Chemical Society, Faraday Transactions, 1997, 93, 2763-2767.	1.7	63
70	Ab initiorate constants from hyperspherical quantum scattering: Application to H+CH4â†'H2+CH3. Journal of Chemical Physics, 2004, 120, 2308-2318.	1.2	63
71	Rovibrational spectra of openâ€shell van der Waals complexes: Arâ€“OH(Xâ€‰2Î). Journal of Chemical Physics, 1991, 94, 4149-4160.	1.2	62
72	Theoretical Study of the Cage Water Hexamer Structure. Journal of Physical Chemistry A, 1997, 101, 6813-6819.	1.1	62

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73	Quantum simulation of the benzene-water complex. Molecular Physics, 1996, 88, 33-52.	0.8	62
74	A comparison of conventional and rigid body diffusion Monte Carlo techniques. Application to water dimer. Chemical Physics Letters, 1994, 228, 547-554.	1.2	61
75	Quantum-mechanical calculations on termolecular association reactions XY+Z+Mâ†'XYZ+M: Application to ozone formation. Journal of Chemical Physics, 2002, 117, 1660-1672.	1.2	61
76	Rate constants for chemical reactions of radicals at low temperatures. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 2185.	1.7	60
77	Timeâ€dependent waveâ€packet studies on the sticking of HCl to an ice surface. Journal of Chemical Physics, 1996, 104, 5663-5673.	1.2	59
78	Calculation of the far-infrared spectra for (HF)2, (HCL)2 and (HBr)2. Chemical Physics Letters, 1991, 187, 345-353.	1.2	58
79	Configuration-interaction-Hylleraas calculations on one-positron atomic systems. Journal of Physics B: Atomic and Molecular Physics, 1976, 9, 3115-3129.	1.6	57
80	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.	1.2	57
81	Vibrational and rotational effects in the Cl+HODâ†"HCl+OD reaction. Journal of Chemical Physics, 1994, 100, 3556-3567.	1.2	57
82	Vibrational relaxation of N2 by collision with He atoms. Journal of Chemical Physics, 1986, 84, 3788-3797.	1.2	56
83	Coupled-channel calculations on energy transfer, photochemistry, and reactions of polyatomic molecules. The Journal of Physical Chemistry, 1987, 91, 1718-1727.	2.9	56
84	Solvation of hydrogen halides on the surface of ice. Faraday Discussions, 1995, 100, 309.	1.6	56
85	Quantum reactive scattering of H + hydrocarbon reactions. Physical Chemistry Chemical Physics, 2006, 8, 917.	1.3	56
86	H-Densities:â€‰ A New Concept for Hydrated Molecules. Accounts of Chemical Research, 2000, 33, 441-447.	7.6	55
87	Quantum free energies of the conformers of glycine on an ab initio potential energy surfaceElectronic supplementary information (ESI) available: Calculated harmonic frequencies of the glycine conformers. See http://www.rsc.org/suppdata/cp/b3/b314644h/. Physical Chemistry Chemical Physics, 2004, 6, 2563.	1.3	55
88	Zero temperature quantum properties of small protonated water clusters (H2O)nH+ (n=1â€"5). Journal of Chemical Physics, 2003, 119, 10048-10062.	1.2	54
89	Quantum Dynamics of Chemical Reactions. Science, 2008, 321, 789-791.	6.0	53
90	Refinement of the OH Aâ€‰2Î£+(v=0)+Ar intermolecular potential energy surface. Journal of Chemical Physics, 1993, 98, 9320-9334.	1.2	52

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91	Quantum scattering on SN2 reactions: Influence of azimuthal rotations. Journal of Chemical Physics, 1998, 109, 8200-8217.	1.2	52
92	Reduced dimensionality quantum dynamics of Cl + CH4? HCl + CH3 on an ab initio potential. Physical Chemistry Chemical Physics, 2007, 9, 933.	1.3	52
93	Theoretical studies on bimolecular reaction dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 12649-12653.	3.3	52
94	Ab initio computation of vibrational relaxation rate coefficients for the collisions of CO2 with helium and neon atoms. Chemical Physics, 1982, 65, 247-257.	0.9	51
95	Quantum-mechanical calculations on pressure and temperature dependence of three-body recombination reactions: Application to ozone formation rates. Journal of Chemical Physics, 2004, 120, 2700-2707.	1.2	51
96	Rate constant calculations on the C++HCl reaction. Journal of Chemical Physics, 1989, 90, 7216-7228.	1.2	50
97	Isotope and potential energy surface effects in vibrational bonding. The Journal of Physical Chemistry, 1984, 88, 2758-2764.	2.9	49
98	Ab initiorate constants from hyperspherical quantum scattering: Application to H+C2H6 and H+CH3OH. Journal of Chemical Physics, 2004, 121, 6809-6821.	1.2	49
99	Kinetic Isotope Effects in the Reactions of D Atoms with CH4, C2H6, and CH3OH: Quantum Dynamics Calculationsâ€. Journal of Physical Chemistry A, 2004, 108, 8966-8972.	1.1	49
100	Variational calculations on many-electron diatomic molecules using Hylleraas-type wavefunctions. Molecular Physics, 1977, 34, 793-811.	0.8	48
101	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.	1.2	48
102	Quantum Simulation of Phenolâ^'Water Clusters. Journal of Physical Chemistry A, 2000, 104, 5590-5599.	1.1	48
103	Weakly bound NeHF. Journal of Chemical Physics, 1989, 91, 711-721.	1.2	47
104	Vibrational predissociation of the Neâ€“C2H4and Arâ€“C2H4van der Waals complexes. Journal of Chemical Physics, 1984, 81, 4474-4480.	1.2	46
105	A full-dimensional quantum dynamical study of vibrational relaxation in H2+H2. Chemical Physics Letters, 2002, 363, 523-528.	1.2	46
106	Classical-trajectory calculations onAr+sputtering of a Si(001) surface using anabinitiopotential. Physical Review B, 1989, 39, 7680-7696.	1.1	45
107	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.	1.2	44
108	Rate Constants for the CH4 + H â†' CH3 + H2 Reaction Calculated with a Generalized Reduced-Dimensionality Method. Journal of Physical Chemistry A, 2002, 106, 8256-8260.	1.1	44

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109	Coupled states calculations on vibrational relaxation in He+CO2(0110) and He+CO. Journal of Chemical Physics, 1987, 86, 802-812.	1.2	43
110	Adsorption of HCL on ice under stratospheric conditions: A computational study. Geophysical Research Letters, 1992, 19, 1355-1358.	1.5	42
111	Reactive scattering of highly vibrationally excited oxygen molecules: Ozone formation?. Journal of Chemical Physics, 1998, 108, 3566-3573.	1.2	42
112	Vibrational predissociation in D2HF. Journal of Chemical Physics, 1992, 96, 90-97.	1.2	41
113	Rotationally inelastic and bound state dynamics of H2-OH(X2Î). Molecular Physics, 1994, 83, 405-428.	0.8	41
114	A new method for calculating the rovibrational states of polyatomics with application to water dimer. Journal of Chemical Physics, 1995, 102, 4390-4399.	1.2	41
115	Application of the vibrationally adiabatic and static distorted wave born approximation of the reaction H + F2(Î½ = 0, j = 0) â† HF(Î½â€²,jâ€²) + F. Chemical Physics Letters, 1979, 66, 493-497.	1.2	40
116	Ab initio calculations on indoleâ€“water, 1-methylindoleâ€“water and indoleâ€“(water)2. Chemical Physics Letters, 2000, 331, 253-261.	1.2	40
117	Mechanism of Photoinduced Changes in the Structure and Optical Properties of AmorphousAs2S3. Physical Review Letters, 2000, 85, 3305-3308.	2.9	40
118	Nuclear quantum effects on the structure and energetics of (H2O)6H+. Physical Chemistry Chemical Physics, 2005, 7, 2324.	1.3	40
119	CI-Hylleraas variational calculation on the ground state of the neon atom. Physical Review A, 1976, 14, 1607-1613.	1.0	39
120	The infiniteâ€orderâ€sudden method for lightâ€“heavyâ€“light reactions: Application to D+HClâ†'DCl+H. Journal of Chemical Physics, 1982, 76, 5027-5033.	1.2	39
121	An ab Initio Calculation of the Low Rotation-Vibration Energies of the CO Dimer. Journal of Molecular Spectroscopy, 1993, 157, 208-219.	0.4	39
122	Molecules on Ice. Science, 1996, 271, 1509-1509.	6.0	39
123	A theory for the photodissociation of polyatomic molecules, with application to CF3I. Journal of Chemical Physics, 1986, 84, 4288-4298.	1.2	38
124	Quantum scattering calculations on the SN2 reaction Clâ¯'+CH3Brâ†'ClCH3+Brâ¯'. Journal of Chemical Physics, 1999, 110, 9483-9491.	1.2	38
125	Product CN Rotational Distributions from the H + HCN Reaction. The Journal of Physical Chemistry, 1995, 99, 13664-13669.	2.9	37
126	Rotational and vibrationalâ€rotational relaxation in collisions of CO2(0110) with He atoms. Journal of Chemical Physics, 1983, 78, 4915-4923.	1.2	36

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127	Potential energy surface effects on differential cross sections for polyatomic reactions. Chemical Physics, 1995, 191, 223-233.	0.9	36
128	A Quantum Study on the Reaction between C(3P) and Acetyleneâ€. Journal of Physical Chemistry A, 2001, 105, 2694-2707.	1.1	36
129	Torsional path integral Monte Carlo method for calculating the absolute quantum free energy of large molecules. Journal of Chemical Physics, 2003, 119, 68-76.	1.2	36
130	Reduced dimensionality spin-orbit dynamics of CH3 + HCl $ightleftharpoons$â‡Œ CH4 + Cl on ab initio surfaces. Journal of Chemical Physics, 2011, 134, 204311.	1.2	36
131	Quantum dynamics in the smallest water droplet. Science, 2016, 351, 1267-1268.	6.0	36
132	Validity of the rotational sudden approximation for vibrational relaxation in He + CO. Chemical Physics Letters, 1983, 101, 269-273.	1.2	35
133	Comparison of variational transition state theory and quantum sudden calculations of threeâ€dimensional rate coefficients for the reactions D(H)+BrHâ€‰â†’â€‰DBr(HBr)+H. Journal of Chemical Physics, 1983, 78, 777-782.	1.2	35
134	Isotopic branching ratio for the O++ HD reaction. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 1685.	1.1	35
135	Rovibrational spectra of openâ€shell van der Waals complexes: H2â€“OH (Xâ€‰2Î). Journal of Chemical Physics, 1993, 98, 1843-1855.	1.2	35
136	Quantum-mechanical study of the resonances of the SN2 reaction Cl-+CH3Clâ†’ClCH3+Cl-. Physical Chemistry Chemical Physics, 1999, 1, 1197-1203.	1.3	35
137	The effect of the symmetric and asymmetric stretching vibrations of CH4 on the O(3P) + CH4â†’OH + CH3 reaction. Physical Chemistry Chemical Physics, 2000, 2, 4105-4114.	1.3	35
138	Low-temperature reactions of He+ and C+ with HCl, SO2 and H2S. Chemical Physics Letters, 1988, 143, 130-134.	1.2	34
139	Improving reduced dimensionality quantum reaction dynamics with a generalized transition state. Application to CH4+O(3P). Journal of Chemical Physics, 2001, 115, 2188-2197.	1.2	34
140	The vibrationally adiabatic distorted wave method for direct chemical reactions: Application to X+F2(v = 0, j = 0)â†’XF(vâ€², jâ€², mjâ€²)+F(X = Mu, H, D, T). Journal of Chemical Physics, 1981, 75, 3329-3339.	1.2	33
141	Rates for the reactions of open-shell ions with molecules. Chemical Physics Letters, 1990, 167, 1-6.	1.2	33
142	Rate constant calculations on the N(4S)+OH(2Î) reaction. Chemical Physics Letters, 2006, 431, 261-266.	1.2	33
143	Hylleraas-type wavefunction for lithium hydride. Chemical Physics Letters, 1977, 51, 483-486.	1.2	32
144	Infrared Spectrum of NeHF. Physical Review Letters, 1988, 61, 1576-1579.	2.9	32

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145	Calculations on vibrational predissociation of Arâ€“OH (Aâ€‰2Î£+). Journal of Chemical Physics, 1991, 95, 8149-8165.	1.2	32
146	Collision-induced conformational changes in glycine. Journal of Chemical Physics, 2005, 122, 244323.	1.2	32
147	Closeâ€coupling calculations on the H+BrHâ†'HBr+H reaction in three dimensions. Journal of Chemical Physics, 1985, 83, 1685-1692.	1.2	31
148	The C6H6â€“(H2O)2 complex: Theoretical predictions of the structure, energetics, and tunneling dynamics. Journal of Chemical Physics, 1997, 106, 849-863.	1.2	31
149	An improved treatment of spectator mode vibrations in reduced dimensional quantum dynamics: Application to the hydrogen abstraction reactions Î¼+CH4, H+CH4, D+CH4, and CH3+CH4. Journal of Chemical Physics, 2009, 131, 044111.	1.2	31
150	Quantum and quasiclassical study of the collinear reaction O(3P) + H2 â†' OH + H using a LEPS and fitted AB initio potential energy surface. Chemical Physics Letters, 1979, 68, 154-157.	1.2	30
151	Fourâ€center reactions: A quantal model for H4. Journal of Chemical Physics, 1996, 104, 8413-8423.	1.2	30
152	Isotopic branching in (He,â€ŠHD+) collisions: A time-dependent quantum mechanical study in three dimensions. Journal of Chemical Physics, 1999, 111, 10910-10918.	1.2	30
153	Torsional diffusion Monte Carlo: A method for quantum simulations of proteins. Journal of Chemical Physics, 2001, 114, 9725-9732.	1.2	30
154	Torsional path integral Monte Carlo method for the quantum simulation of large molecules. Journal of Chemical Physics, 2002, 116, 8262.	1.2	30
155	Distorted-wave calculations for the three dimensional chemical reaction H + H2(v â©½ 2, j = 0) â†' H2(vâ€² â©½ 2, jâ€²,) Tj ETQq1	0.9	29
156	New quantum-dynamical approximation for light-heavy-light chemical reactions in three dimensions theory. Molecular Physics, 1981, 44, 1067-1081.	0.8	29
157	Propensity rules in rotationally inelastic collisions of CO2. Chemical Physics Letters, 1983, 98, 319-323.	1.2	29
158	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.	2.2	29
159	The O(3P) + H2(Î½ â©½2, j, mj) â†'OH(Î½â€² â©½2, jâ€², mjâ€²) + H reaction. Molecular Physics, 1980, 41, 689-702.	0.8	28
160	Iterative solution in quantum scattering theory. The log derivative Kohn approach. Journal of the Chemical Society, Faraday Transactions, 1990, 86, 1641.	1.7	28
161	Diffusion Monte Carlo studies of isotope-substituted water trimers. Chemical Physics Letters, 1996, 263, 680-686.	1.2	28
162	Isotope Effects in the Formation of Molecular Hydrogen on a Graphite Surface via an Eleyâ^'Rideal Mechanism. Journal of Physical Chemistry A, 2002, 106, 8996-9008.	1.1	28

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163	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.	1.2	28
164	New quantum-dynamical approximation for light-heavy-light chemical reactions in three dimensions. Molecular Physics, 1981, 44, 1083-1097.	0.8	27
165	Comparison of the Floquet and rotating-wave methods for multiphoton excitation of sulfur hexafluoride. The Journal of Physical Chemistry, 1983, 87, 735-739.	2.9	27
166	Rate constants of chemical reactions from semiclassical transition state theory in full and one dimension. Journal of Chemical Physics, 2016, 144, 244116.	1.2	27
167	New Developments in Semiclassical Transition-State Theory. Journal of Physical Chemistry A, 2019, 123, 4639-4657.	1.1	27
168	A theory for Coriolis enhanced vibrational energy transfer and its application to D2CO + rare gas collisions. Molecular Physics, 1986, 59, 529-545.	0.8	26
169	Vibrational energy transfer in collisions of He atoms with paraâ€difluorobenzene. Journal of Chemical Physics, 1987, 86, 813-821.	1.2	26
170	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.	1.2	26
171	Quaternion formulation of diffusion quantum Monte Carlo for the rotation of rigid molecules in clusters. Journal of Chemical Physics, 2000, 113, 5193.	1.2	26
172	Quantum scattering study of the abstraction reactions of H atoms from CH3NH2. Chemical Physics Letters, 2007, 438, 1-7.	1.2	26
173	Reduced Dimensionality Quantum Dynamics of CH₃ + CH₄ â†' CH₄ + CH₃: Symmetric Hydrogen Exchange on an Ab Initio Potential. Journal of Physical Chemistry A, 2009, 113, 4255-4264.	1.1	26
174	The significance of fermi resonance for the collisions of triatomic molecules with atoms. Chemical Physics Letters, 1980, 74, 454-458.	1.2	25
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