List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	From six to eight Î-electron bare rings of group-XIV elements and beyond: can planarity be deciphered from the "quasi-molecules―they embed?. Physical Chemistry Chemical Physics, 2022, 24, 8488-8507.	2.8	5
2	Quasiclassical Trajectory Study of the Si + SH Reaction on an Accurate Double Many-Body Expansion Potential Energy Surface. Journal of Physical Chemistry A, 2022, 126, 3555-3568.	2.5	2
3	Post-complete-basis-set extrapolation of conventional and explicitly correlated coupled-cluster energies: can the convergence to the CBS limit be diagnosed?. Physical Chemistry Chemical Physics, 2021, 23, 8717-8730.	2.8	10
4	Canonical and explicitly-correlated coupled cluster correlation energies of sub-kJ mol ^{â^1} accuracy <i>via</i> cost-effective hybrid-post-CBS extrapolation. Physical Chemistry Chemical Physics, 2021, 23, 9571-9584.	2.8	12
5	Accurate DMBE potential-energy surface for CNO(2 <i>A</i> ″) and rate coefficients in C(3P)+NO collisions. Journal of Chemical Physics, 2021, 154, 034303.	3.0	3
6	Modelling adiabatic cusps in via 2 × 2 diabatic matrix. Molecular Physics, 2021, 119, e1904157.	1.7	5
7	SiS Formation in the Interstellar Medium through Si+SH Gas-phase Reactions. Astrophysical Journal, 2021, 920, 37.	4.5	10
8	Optimized Structural Data at the Complete Basis Set Limit via Successive Quadratic Minimizations. Journal of Physical Chemistry A, 2021, 125, 10657-10666.	2.5	5
9	Extrapolation in quantum chemistry: Insights on energetics and reaction dynamics. Journal of Theoretical and Computational Chemistry, 2020, 19, 2030001.	1.8	11
10	Accurate Potential Energy Surface for Quartet State HN ₂ and Interplay of N(⁴ <i>S</i>) + NH(<i>XÌf</i> ³ Σ [–]) versus H + N ₂ (<i>A</i> ³ Σ _u ⁺) Reactions. Journal of Physical Chemistry A, 2020, 124, 781-789.	2.5	5
11	Effect of initial vibrational excitation on the methane cation sub-femtosecond photodynamics. Molecular Physics, 2020, 118, e1752403.	1.7	0
12	Quasiclassical Study of the C(³ P) + NO(X ² Î) and O(³ P) + CN(X ² Σ ⁺) Collisional Processes on an Accurate DMBE Potential Energy Surface. Journal of Physical Chemistry A, 2019, 123, 7195-7200.	2.5	7
13	Global Potential Energy Surface for HO ₂ ⁺ Using the CHIPR Method. Journal of Physical Chemistry A, 2019, 123, 1613-1621.	2.5	8
14	Accurate CHIPR Potential Energy Surface for the Lowest Triplet State of C _{3} . Journal of Physical Chemistry A, 2019, 123, 8154-8169.	2.5	13
15	Optimal basis sets for CBS extrapolation of the correlation energy: oV <i>x</i> Z and oV(<i>x</i> + <i>d</i>)Z. Journal of Chemical Physics, 2019, 150, 154106.	3.0	2
16	CBS extrapolation of Hartree–Fock energy: Pople and Dunning basis sets hand-to-hand on the endeavour. Physical Chemistry Chemical Physics, 2019, 21, 8022-8034.	2.8	15
17	A global CHIPR potential energy surface for ground-state C ₃ H and exploratory dynamics studies of reaction C ₂ + CH → C ₃ + H. Physical Chemistry Chemical Physics, 2019, 21, 24406-24418.	2.8	11
18	Difficulties and Virtues in Assessing the Potential Energy Surfaces of Carbon Clusters via DMBE Theory: Stationary Points of C _{l̂≤} (l̂º = 2–10) at the Focal Point. Journal of Physical Chemistry A, 2019, 123, 3121-3130.	2.5	5

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19	Accurate Explicit-Correlation-MRCI-Based DMBE Potential-Energy Surface for Ground-State CNO. Journal of Physical Chemistry A, 2018, 122, 4198-4207.	2.5	13
20	<i>C</i> _{<i>n</i>} (<i>n</i> =2â^'4): current status. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2018, 376, 20170145.	3.4	21
21	Multiple conical intersections in small linear parameter Jahn–Teller systems: the DMBE potential energy surface of ground-state C ₃ revisited. Physical Chemistry Chemical Physics, 2018, 20, 10319-10331.	2.8	6
22	The O + NO(<i>v</i>) Vibrational Relaxation Processes Revisited. Journal of Physical Chemistry A, 2018, 122, 5299-5310.	2.5	10
23	CBS extrapolation in electronic structure pushed to the end: a revival of minimal and sub-minimal basis sets. Physical Chemistry Chemical Physics, 2018, 20, 22084-22098.	2.8	25
24	The Jahn-Teller plus pseudo-Jahn-Teller vibronic problem in the C3 radical and its topological implications. Journal of Chemical Physics, 2016, 144, 064309.	3.0	19
25	Extrapolation of Hartree–Fock and multiconfiguration self-consistent-field energies to the complete basis set limit. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	28
26	Structural evolution of the methane cation in subfemtosecond photodynamics. Journal of Chemical Physics, 2015, 143, 014304.	3.0	17
27	Application of the Unified Singlet and Triplet Electron-Pair Extrapolation Scheme with Basis Set Rehierarchization to Tensorial Properties. Journal of Physical Chemistry A, 2015, 119, 1208-1217.	2.5	14
28	Modeling Cusps in Adiabatic Potential Energy Surfaces. Journal of Physical Chemistry A, 2015, 119, 1415-1421.	2.5	15
29	Subfemtosecond Quantum Nuclear Dynamics in Water Isotopomers. Journal of Physical Chemistry A, 2015, 119, 4856-4863.	2.5	7
30	Sub-femtosecond quantum dynamics of the strong-field ionization of water to the XÌf ² B ₁ and Ãf ² A ₁ states of the cation. Physical Chemistry Chemical Physics, 2015, 17, 6545-6553.	2.8	8
31	Effect of Initial Vibrational-State Excitation on Subfemtosecond Photodynamics of Water. Journal of Physical Chemistry A, 2015, 119, 12367-12375.	2.5	4
32	Accurate <i>ab initio</i> -based double many-body expansion potential energy surface for the adiabatic ground-state of the C3 radical including combined Jahn-Teller plus pseudo-Jahn-Teller interactions. Journal of Chemical Physics, 2015, 143, 074302.	3.0	19
33	Dynamics of the O + ClO Reaction: Reactive and Vibrational Relaxation Processes. Journal of Physical Chemistry A, 2014, 118, 12120-12129.	2.5	1
34	Narrowing the error in electron correlation calculations by basis set re-hierarchization and use of the unified singlet and triplet electron-pair extrapolation scheme: Application to a test set of 106 systems. Journal of Chemical Physics, 2014, 141, 224113.	3.0	76
35	Exploring the Utility of Many-Body Expansions: A Consistent Set of Accurate Potentials for the Lowest Quartet and Doublet States of the Azide Radical with Revisited Dynamics. Journal of Physical Chemistry A, 2014, 118, 10127-10133.	2.5	6
36	Is HO3â^' multiple-minimum and floppy? Covalent to van der Waals isomerization and bond rupture of a peculiar anion. Physical Chemistry Chemical Physics, 2014, 16, 16997-17007.	2.8	5

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37	On Extracting Subfemtosecond Data from Femtosecond Quantum Dynamics Calculations: The Methane Cation. Journal of Chemical Theory and Computation, 2014, 10, 3606-3616.	5.3	20
38	Electronic Quenching in N(² D) + N ₂ Collisions: A State-Specific Analysis via Surface Hopping Dynamics. Journal of Chemical Theory and Computation, 2014, 10, 1872-1877.	5.3	16
39	Single-Sheeted Double Many-Body Expansion Potential Energy Surface for Ground-State ClO ₂ . Journal of Physical Chemistry A, 2014, 118, 4851-4862.	2.5	6
40	Roadmap to spline-fitting potentials in high dimensions. Journal of Mathematical Chemistry, 2013, 51, 1729-1746.	1.5	15
41	Silane Radical Cation: A Theoretical Account on the Jahn–Teller Effect at a Triple Degeneracy. Journal of Physical Chemistry A, 2013, 117, 8794-8805.	2.5	3
42	Accurate Determination of the Reaction Course in HY ₂ ⇌ Y + YH (Y = O, S): Detailed Analysis of the Covalent- to Hydrogen-Bonding Transition. Journal of Physical Chemistry A, 2013, 117, 7393-7407.	2.5	16
43	Combined-hyperbolic-inverse-power-representation of potential energy surfaces: A preliminary assessment for H3 and HO2. Journal of Chemical Physics, 2013, 138, 054120.	3.0	36
44	Accurate Study of the Two Lowest Singlet States of HN ₃ : Stationary Structures and Energetics at the MRCI Complete Basis Set Limit. Journal of Physical Chemistry A, 2013, 117, 4044-4050.	2.5	7
45	Electronic Quenching of N(² D) by N ₂ : Theoretical Predictions, Comparison with Experimental Rate Constants, and Impact on Atmospheric Modeling. Journal of Physical Chemistry Letters, 2013, 4, 2292-2297.	4.6	22
46	Accurate combined-hyperbolic-inverse-power-representation of <i>ab initio</i> potential energy surface for the hydroperoxyl radical and dynamics study of \$f O+OH\$O+OH reaction. Journal of Chemical Physics, 2013, 138, 134117.	3.0	36
47	Manifestation of external field effect in time-resolved photo-dissociation dynamics of LiF. Chinese Physics B, 2013, 22, 073303.	1.4	2
48	Implications of the O + OH reaction in hydroxyl nightglow modeling. Atmospheric Chemistry and Physics, 2013, 13, 1-13.	4.9	60
49	Quadratic coupling treatment of the Jahn-Teller effect in the triply-degenerate electronic state of \$f CH_4^+\$CH4+: Can one account for floppiness?. Journal of Chemical Physics, 2012, 137, 214320.	3.0	12
50	N(4 <i>S</i> /2 <i>D</i>)+N2: Accurate <i>ab initio</i> -based DMBE potential energy surfaces and surface-hopping dynamics. Journal of Chemical Physics, 2012, 137, 22A515.	3.0	27
51	<i>Ab Initio</i> Treatment of Bond-Breaking Reactions: Accurate Course of HO ₃ Dissociation and Revisit to Isomerization. Journal of Chemical Theory and Computation, 2012, 8, 428-441.	5.3	45
52	Ab Initio-Based Global Double Many-Body Expansion Potential Energy Surface for the First 2A″ Electronic State of NO2. Journal of Physical Chemistry A, 2012, 116, 3023-3034.	2.5	17
53	Dynamics study of a three-fold pseudo-Jahn–Teller system using the extended Longuet–Higgins formalism. Journal of Chemical Sciences, 2012, 124, 115-120.	1.5	0
54	Toward the modeling of the NO ₂ (² <i>A</i> [″]) manifold. International Journal of Quantum Chemistry, 2011, 111, 3776-3785.	2.0	12

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55	Anatomy of the S(1D) + H2 reaction: the dynamics on two new potential energy surfaces from quantum dynamics calculations. Physical Chemistry Chemical Physics, 2011, 13, 13645.	2.8	26
56	ls HO3 minimum cis or trans? An analytic full-dimensional ab initio isomerization path. Physical Chemistry Chemical Physics, 2011, 13, 9796.	2.8	35
57	Accurate Double Many-Body Expansion Potential Energy Surface for Ground-State HS ₂ Based on ab Initio Data Extrapolated to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2011, 115, 5274-5283.	2.5	30
58	Quasiclassical Trajectory Study of the C(¹ <i>D</i>) + H ₂ Reaction and Isotopomeric Variants: Kinetic Isotope Effect and CD/CH Branching Ratio. Journal of Physical Chemistry A, 2011, 115, 7882-7890.	2.5	25
59	Ab Initio Based Double-Sheeted DMBE Potential Energy Surface for N ₃ (² <i>A</i> ″) and Exploratory Dynamics Calculations. Journal of Physical Chemistry A, 2011, 115, 12390-12398.	2.5	26
60	Generalized Born–Oppenheimer treatment of Jahn–Teller systems in Hilbert spaces of arbitrary dimension: theory and application to a three-state model potential. Physical Chemistry Chemical Physics, 2011, 13, 8131.	2.8	13
61	On the stability of the elusive HO3 radical. Physical Chemistry Chemical Physics, 2011, 13, 15619.	2.8	37
62	The Jahn-Teller effect in the triply degenerate electronic state of methane radical cation. Journal of Chemical Physics, 2011, 135, 174304.	3.0	24
63	Heliumâ€fullerene pair interactions: An ab initio study by perturbation theory and coupled cluster methods. International Journal of Quantum Chemistry, 2011, 111, 416-429.	2.0	14
64	Quasiclassical trajectory study of the rotational distribution for the O+NO(<i>v</i> = 0) fundamental vibrational excitation. International Journal of Chemical Kinetics, 2011, 43, 345-352.	1.6	3
65	Quantum calculations for the S(1D)+H2reaction employing the ground adiabatic electronic state. Physica Scripta, 2011, 84, 028102.	2.5	14
66	On the role of dynamical barriers in barrierless reactions at low energies: S(1 <i>D</i>) + H2. Journal of Chemical Physics, 2011, 135, 134313.	3.0	26
67	Spin-component-scaling second-order MÃ,ller–Plesset theory and its variants for economical correlation energies: Unified theoretical interpretation and use for quartet N3. Journal of Chemical Physics, 2010, 133, 064104.	3.0	16
68	Extrapolation to the Complete Basis Set Limit without Counterpoise. The Pair Potential of Helium Revisited ^{â€} . Journal of Physical Chemistry A, 2010, 114, 8505-8516.	2.5	69
69	Ab Initio Study of Hydrazinyl Radical: Toward a DMBE Potential Energy Surface. Journal of Physical Chemistry A, 2010, 114, 11663-11669.	2.5	3
70	Quasiclassical Trajectory Study of Atom-Exchange and Vibrational Relaxation Processes in Collisions of Atomic and Molecular Nitrogen. Journal of Physical Chemistry A, 2010, 114, 6063-6070.	2.5	28
71	Accurate MRCI and CC Study of the Most Relevant Stationary Points and Other Topographical Attributes for the Ground-State C ₂ H ₂ Potential Energy Surface. Journal of Physical Chemistry A, 2010, 114, 13277-13287.	2.5	24
72	Ab-Initio-Based Global Double Many-Body Expansion Potential Energy Surface for the Electronic Ground State of the Ammonia Molecule. Journal of Physical Chemistry A, 2010, 114, 6669-6680.	2.5	22

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73	Accurate Potential Energy Surface for the 1 ² A′ State of NH ₂ : Scaling of External Correlation Versus Extrapolation to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2010, 114, 9644-9654.	2.5	29
74	Ab initio Based DMBE Potential Energy Surface for the Ground Electronic State of the C ₂ H Molecule. Journal of Physical Chemistry A, 2010, 114, 2655-2664.	2.5	7
75	Accurate Double Many-Body Expansion Potential Energy Surface for N ₃ (⁴ A′′) from Correlation Scaled ab Initio Energies with Extrapolation to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2009, 113, 14424-14430.	2.5	51
76	DIABATIC ELECTRONIC MANIFOLD OF HN ₂ (² A′) AND N + NH REACTION DYNAMICS ON ITS LOWEST ADIABAT. Journal of Theoretical and Computational Chemistry, 2009, 08, 849-859.	1.8	11
77	Accurate <i>ab initio</i> potential energy curves for the classic Li–F ionic-covalent interaction by extrapolation to the complete basis set limit and modeling of the radial nonadiabatic coupling. Journal of Chemical Physics, 2009, 131, 124128.	3.0	62
78	MÃ,ller–Plesset perturbation energies and distances for HeC ₂₀ extrapolated to the complete basis set limit. Journal of Computational Chemistry, 2009, 30, 379-388.	3.3	15
79	Theoretical study of the O + HSO reaction. International Journal of Chemical Kinetics, 2009, 41, 455-462.	1.6	4
80	Potential Energy Surface for Ground-State H2S via Scaling of the External Correlation, Comparison with Extrapolation to Complete Basis Set Limit, and Use in Reaction Dynamics. Journal of Physical Chemistry A, 2009, 113, 9213-9219.	2.5	25
81	Accurate <i>ab initio</i> based DMBE potential energy surface for the ground electronic state of N2H2. Journal of Chemical Physics, 2009, 131, 044309.	3.0	27
82	Accurate <i>ab initio</i> double many-body expansion potential energy surface for ground-state H2S by extrapolation to the complete basis set limit. Journal of Chemical Physics, 2009, 130, 134317.	3.0	50
83	Accurate Double Many-Body Expansion Potential Energy Surface for the Lowest Singlet State of Methylene. Journal of Physical Chemistry A, 2009, 113, 4175-4183.	2.5	21
84	Can extrapolation to the basis set limit be an alternative to the counterpoise correction? A study on the helium dimer. Theoretical Chemistry Accounts, 2008, 119, 511-521.	1.4	40
85	Dynamics and kinetics of the S + HO ₂ reaction: A theoretical study. International Journal of Chemical Kinetics, 2008, 40, 533-540.	1.6	7
86	Extrapolation to the complete-basis-set limit and the implications of avoided crossings: The X Σ1g+, B Δ and B′ Σ1g+ states of C2. Journal of Chemical Physics, 2008, 129, 234103.	¹ g:o	60
87	A Theoretical Study of Rate Coefficients for the O + NO Vibrational Relaxation. Journal of Physical Chemistry A, 2008, 112, 960-965.	2.5	12
88	Extrapolating to the One-Electron Basis Set Limit in Polarizability Calculations. Journal of Physical Chemistry A, 2008, 112, 10413-10419.	2.5	15
89	Generalized Uniform Singlet- and Triplet-Pair Extrapolation of the Correlation Energy to the One Electron Basis Set Limit. Journal of Physical Chemistry A, 2008, 112, 1841-1850.	2.5	40
90	Energy-switching potential energy surface for the water molecule revisited: A highly accurate singled-sheeted form. Journal of Chemical Physics, 2008, 129, 044302.	3.0	11

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91	Intermolecular and Intramolecular Potentials: Topographical Aspects, Calculation, and Functional Representation via A Double Many-Body Expansion Method. Advances in Chemical Physics, 2007, , 255-338.	0.3	160
92	Accurate <i>ab initio</i> potentials at low cost via correlation scaling and extrapolation: Application to CO(AÎ1). Journal of Chemical Physics, 2007, 127, 114316.	3.0	45
93	Accurate <i>ab initio</i> -based molecular potentials: from extrapolation methods to global modelling. Physica Scripta, 2007, 76, C28-C35.	2.5	23
94	Recalibrated Double Many-Body Expansion Potential Energy Surface and Dynamics Calculations for HN2. Journal of Physical Chemistry A, 2007, 111, 1172-1178.	2.5	24
95	Extrapolating to the one-electron basis-set limit in electronic structure calculations. Journal of Chemical Physics, 2007, 126, 244105.	3.0	176
96	Kinetics and dynamics of O + OClO reaction in a modified many-body expansion potential energy surface for ClO3. International Journal of Chemical Kinetics, 2007, 39, 422-430.	1.6	0
97	Predicting Catalysis:Â Understanding Ammonia Synthesis from First-Principles Calculations. Journal of Physical Chemistry B, 2006, 110, 17719-17735.	2.6	192
98	Dynamics of X+CH4 (X=H,O,Cl) reactions: How reliable is transition state theory for fine-tuning potential energy surfaces?. Journal of Chemical Physics, 2006, 125, 064312.	3.0	38
99	New Double Many-Body Expansion Potential Energy Surface for Ground-State HCN from a Multiproperty Fit to Accurate ab Initio Energies and Rovibrational Calculationsâ€. Journal of Physical Chemistry A, 2006, 110, 485-493.	2.5	43
100	Accurate DMBE Potential Energy Surface For the N(2D) + H2(1Σ g +) Reaction Using an Improved Switching Function Formalism. Theoretical Chemistry Accounts, 2006, 116, 404-419.	1.4	73
101	What are the Implications of Nonequilibrium in the O+OH and O+HO2 Reactions?. ChemPhysChem, 2005, 6, 453-465.	2.1	19
102	Double many-body expansion potential energy surface for ground state HSO2. Physical Chemistry Chemical Physics, 2005, 7, 2305.	2.8	56
103	Repulsive double many-body expansion potential energy surface for the reactions N(4S)+ H2⇌ NH(X3Σ–)+ H from accurate ab initio calculations. Physical Chemistry Chemical Physics, 2005, 7, 2867.	2.8	44
104	Reply to the Comment on "Are Vibrationally Excited Molecules a Clue for the O3Deficit Problem and HOxDilemma in the Middle Atmosphere?― Journal of Physical Chemistry A, 2005, 109, 2700-2702.	2.5	8
105	Unimolecular and Bimolecular Calculations for HN2. Journal of Physical Chemistry A, 2005, 109, 2356-2363.	2.5	50
106	MODELING AND INTERPOLATION OF GLOBAL MULTI-SHEETED POTENTIAL ENERGY SURFACES. Advanced Series in Physical Chemistry, 2004, , 205-270.	1.5	28
107	Geometric phase effect at N -fold electronic degeneracies in Jahn-Teller systems. International Journal of Quantum Chemistry, 2004, 99, 385-392.	2.0	5
108	Dynamics study of ClO + O2collisions and their role in the chemistry of stratospheric ozone. Physical Chemistry Chemical Physics, 2004, 6, 2179-2184.	2.8	5

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109	Dynamics Study of the N(4S) + O2Reaction and Its Reverse. Journal of Physical Chemistry A, 2004, 108, 3556-3564.	2.5	36
110	Are Vibrationally Excited Molecules a Clue for the "O3Deficit Problem―and "HOxDilemma―in the Middle Atmosphere?. Journal of Physical Chemistry A, 2004, 108, 758-769.	2.5	39
111	Nascent versus "Steady-State―Rovibrational Distributions in the Products of the O(3P) + O3(X̃1A) Reaction. Journal of Physical Chemistry A, 2003, 107, 10926-10932.	2.5	2
112	Accurate Single-Valued Double Many-Body Expansion Potential Energy Surface for Ground-State HN2. Journal of Physical Chemistry A, 2003, 107, 7923-7930.	2.5	38
113	Steady-State Distributions of O2 and OH in the High Atmosphere and Implications in the Ozone Chemistry. Journal of Physical Chemistry A, 2003, 107, 3769-3777.	2.5	19
114	Dynamics Study of the Reaction S + O2 → SO + O and Its Reverse on a Single-Valued Double Many-Body Expansion Potential Energy Surface for Ground-State SO2. Journal of Physical Chemistry A, 2003, 107, 5369-5374.	2.5	13
115	A realistic multi-sheeted potential energy surface for NO2(2A′) from the double many-body expansion method and a novel multiple energy-switching scheme. Journal of Chemical Physics, 2003, 119, 2596-2613.	3.0	46
116	Permutational Symmetry and the Role of Nuclear Spin in the Vibrational Spectra of Molecules in Doubly Degenerate Electronic States: The Trimers of 2 S Atoms. Advances in Chemical Physics, 2003, , 659-741.	0.3	3
117	On the Geometric Phase Effect in Jahn-Teller Systems. , 2003, , 707-766.		0
118	Li + Li2 Dissociation Reaction Using the Self-Consistent Potential and Trajectory Surface Hopping Methods. Journal of Physical Chemistry A, 2002, 106, 3673-3680.	2.5	1
119	Single-Valued Double Many-Body Expansion Potential Energy Surface of Ground-State SO2. Journal of Physical Chemistry A, 2002, 106, 556-562.	2.5	27
120	Dynamics Study of the OH + O2Branching Atmospheric Reaction. 4. Influence of Vibrational Relaxation in Collisions Involving Highly Excited Species. Journal of Physical Chemistry A, 2002, 106, 5314-5322.	2.5	17
121	DYNAMICS OF O + O3 REACTION ON A NEW POTENTIAL ENERGY SURFACE FOR GROUND-TRIPLET TETRAOXYGEN: SPECTATOR BOND MECHANISM REVISITED. Journal of Theoretical and Computational Chemistry, 2002, 01, 31-43.	1.8	11
122	Dynamics of OH + O2vibrational relaxation processes. Physical Chemistry Chemical Physics, 2002, 4, 4959-4969.	2.8	17
123	Dynamics Study of the O2 + HO2 Atmospheric Reaction with Both Reactants Highly Vibrationally Excited. Journal of Physical Chemistry A, 2002, 106, 11911-11916.	2.5	6
124	A VTST Study of the H + O3and O + HO2Reactions Using a Six-dimensional DMBE Potential Energy Surface for Ground State HO3. Journal of Physical Chemistry A, 2002, 106, 4077-4083.	2.5	23
125	A realistic double many-body expansion potential energy surface for from a multiproperty fit to accurate ab initio energies and vibrational levels. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 629-647.	3.9	34
126	Dynamics of the OH(v = 1,2,4) + O3 atmospheric reaction. Physical Chemistry Chemical Physics, 2001, 3, 1439-1445.	2.8	22

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127	Single-Valued DMBE Potential Energy Surface for HSO:Â A Distributedn-Body Polynomial Approach. Journal of Physical Chemistry A, 2001, 105, 5923-5932.	2.5	64
128	Dynamics Study of the OH + O2 Branching Atmospheric Reaction. 3. Dissociation in Collisions of Vibrationally Excited Reactants. Journal of Physical Chemistry A, 2001, 105, 7435-7440.	2.5	10
129	Vibrational Calculations for the HD2First-Excited Electronic State Using a Coordinate-Transformation Techniqueâ€. Journal of Physical Chemistry A, 2001, 105, 2246-2250.	2.5	8
130	Dynamics Study of the OH + O2 Branching Atmospheric Reaction. 2. Influence of Reactants Internal Energy in HO2 and O3 Formation. Journal of Physical Chemistry A, 2001, 105, 4395-4402.	2.5	20
131	Nuclear dynamics in the vicinity of a crossing seam: Vibrational spectrum of HD2 revisited. International Journal of Quantum Chemistry, 2001, 83, 279-285.	2.0	3
132	Reply to the †Comment on "On the high pressure rate constants for the H/Mu + O2 addition reactions''' by L. B. Harding, J. Troe and V. G. Ushakov, Phys. Chem. Chem. Phys., 2001, 3, 2630. Physical Chemistry Chemical Physics, 2001, 3, 2632-2633.	2.8	15
133	Geometric phase effect in isotopomers of X3 systems: Use of a split basis technique for the cone states of HD2. International Journal of Quantum Chemistry, 2000, 80, 454-460.	2.0	6
134	Basis-set extrapolation of the correlation energy. Journal of Chemical Physics, 2000, 113, 8880-8887.	3.0	151
135	Nuclear dynamics in the vicinity of the crossing seam: Theory and application to vibrational spectrum of H3. Journal of Chemical Physics, 2000, 112, 2121-2127.	3.0	46
136	Coupled <i>ab initio</i> potential energy surfaces for the two lowest ² A′ electronic states of the C ₂ H molecule. Molecular Physics, 2000, 98, 1925-1938.	1.7	8
137	On the variation of the electric quadrupole moment with internuclear distance and the atom–diatom long-range electrostatic interaction energy. Physical Chemistry Chemical Physics, 2000, 2, 435-439.	2.8	18
138	lsotope effect on unimolecular dissociation of MuO2: a classical trajectory study. Physical Chemistry Chemical Physics, 2000, 2, 3583-3589.	2.8	6
139	Four-atom bimolecular reactions with relevance in environmental chemistry: Theoretical work. International Reviews in Physical Chemistry, 2000, 19, 199-245.	2.3	82
140	MRCI Calculation, Scaling of the External Correlation, and Modeling of Potential Energy Curves for HCl and OCl. Journal of Physical Chemistry A, 2000, 104, 6241-6246.	2.5	9
141	Vibrational spectrum of ground state Li ₃ and statistical analysis of the energy levels. Molecular Physics, 1999, 96, 1193-1206.	1.7	15
142	Vibrational spectrum of Li3 first-excited electronic doublet state: Geometric-phase effects and statistical analysis. International Journal of Quantum Chemistry, 1999, 75, 89-109.	2.0	17
143	Comparative trajectory surface hopping study for the Li+Li2(X1Σg+), Na+Li2(X1Σg+) and Li+Na2(X1Σg+) dissociation reactions. Physical Chemistry Chemical Physics, 1999, 1, 2657-2665.	2.8	1
144	Monte Carlo Simulation Approach to Internal Partition Functions for van der Waals Molecules. Journal of Physical Chemistry A, 1999, 103, 8303-8308.	2.5	11

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145	Dynamics Study of the HO(vâ€~=0) + O2(vâ€~Ââ€~) Branching Atmospheric Reaction. 1. Formation of Hydroperoxyl Radical. Journal of Physical Chemistry A, 1999, 103, 4815-4822.	2.5	16
146	On the Rate Constant for the Association Reaction H + CN + Ar → HCN + Ar. Journal of Physical Chemistry A, 1999, 103, 6366-6372.	2.5	7
147	Approximate Quantum Mechanical Cross Sections and Rate Constants for the H + O3 Atmospheric Reaction Using Novel Elastic Optimum Angle Adiabatic Approaches. Journal of Physical Chemistry A, 1999, 103, 1967-1971.	2.5	15
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