AntÃ³nio J C Varandas

List of Publications by Year
in descending order

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409	10,889	41627	78623
papers	citations	51 h-index	77 g-index

421	421	421	3533
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	From six to eight Ï-electron bare rings of group-XIV elements and beyond: can planarity be deciphered from the â€œquasi-moleculesâ€•they embed?. Physical Chemistry Chemical Physics, 2022, 24, 8488-8507.	1.3	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.	1.1	2
3	On the solvation model and infrared spectroscopy of liquid water. Chemical Physics Letters, 2022, 801, 139739.	1.2	3
4	MP2 versus density functional theory calculations in CO 2 â€sequestration reactions with anions: Basis set extrapolation and solvent effects. International Journal of Quantum Chemistry, 2021, 121, e26583.	1.0	4
5	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.	1.3	10
6	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.	1.3	12
7	Accurate DMBE potential-energy surface for CNO(2<i>A</i>â€³) and rate coefficients in C(3P)+NO collisions. Journal of Chemical Physics, 2021, 154, 034303.	1.2	3
8	A general code for fitting global potential energy surfaces via CHIPR method: Direct-Fit Diatomic and tetratomic molecules. Computer Physics Communications, 2021, 258, 107556.	3.0	15
9	Modelling adiabatic cusps in via 2 Ã— 2 diabatic matrix. Molecular Physics, 2021, 119, e1904157.	0.8	5
10	Quantum and Classical Dynamics of the N(²D) + N₂ Reaction on Its Ground Doublet State N₃(1²Aâ€³) Potential Energy Surface. Journal of Physical Chemistry A, 2021, 125, 5650-5660.	1.1	3
11	A further look at the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si40.svg"><mml:mrow><mml:mi mathvariant="normal">Li</mml:mi><mml:mo linebreak="badbreak">+</mml:mo><mml:mi mathvariant="normal">HCl</mml:mi><mml:mo>â†’</mml:mo><mml:mi mathvariant="normal">LiCl</mml:mi><mml:mo linebreak="badbreak">+</mml:mo><mml:mi mathvariant="normal">H</mml:mi></mml:mrow></mml:math> reaction. Chemical Physics Letters, 2021,	1.2	1
12	Dynamical calculations of O(³P) + OH(²Î) reaction on the CHIPR potential energy surface using the fully coupled time-dependent wave-packet approach in hyperspherical coordinates. Physical Chemistry Chemical Physics, 2021, 23, 21784-21796.	1.3	2
13	Canonical versus explicitly correlated coupled cluster: Postâ€completeâ€basisâ€set extrapolation and the quest of the completeâ€basisâ€set limit. International Journal of Quantum Chemistry, 2021, 121, e26598.	1.0	12
14	SiS Formation in the Interstellar Medium through Si+SH Gas-phase Reactions. Astrophysical Journal, 2021, 920, 37.	1.6	10
15	Optimized Structural Data at the Complete Basis Set Limit via Successive Quadratic Minimizations. Journal of Physical Chemistry A, 2021, 125, 10657-10666.	1.1	5
16	A general code for fitting global potential energy surfaces via CHIPR method: Triatomic molecules. Computer Physics Communications, 2020, 247, 106913.	3.0	16
17	Binding of muonated hydrogen molecules and Bornâ€“Oppenheimer approximation revisited. Canadian Journal of Physics, 2020, 98, 379-384.	0.4	2
18	Optimal diffuse augmented atomic basis sets for extrapolation of the correlation energy. International Journal of Quantum Chemistry, 2020, 120, e26135.	1.0	1

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19	Role of Augmented Basis Sets and Quest for ab Initio Performance/Cost Alternative to Kohnâ€“Sham Density Functional Theory. Journal of Physical Chemistry A, 2020, 124, 126-134.	1.1	9
20	Extrapolation in quantum chemistry: Insights on energetics and reaction dynamics. Journal of Theoretical and Computational Chemistry, 2020, 19, 2030001.	1.8	11
21	Accurate Potential Energy Surface for Quartet State HN₂ and Interplay of N(⁴S) + NH(Xìf³Î£^{â€“}) versus H + N₂(A³Î£_u⁺) Reactions. Journal of Physical Chemistry A, 2020, 124, 781-789.	1.1	5
22	Effect of initial vibrational excitation on the methane cation sub-femtosecond photodynamics. Molecular Physics, 2020, 118, e1752403.	0.8	0
23	Quasiclassical Study of the C(³P) + NO(X²Î) and O(³P) + CN(X²Î£⁺) Collisional Processes on an Accurate DMBE Potential Energy Surface. Journal of Physical Chemistry A, 2019, 123, 7195-7200.	1.1	7
24	Fully coupled (J > 0) time-dependent wave-packet calculations using hyperspherical coordinates for the H + O₂ reaction on the CHIPR potential energy surface. Physical Chemistry Chemical Physics, 2019, 21, 20166-20176.	1.3	13
25	Global Potential Energy Surface for HO₂⁺ Using the CHIPR Method. Journal of Physical Chemistry A, 2019, 123, 1613-1621.	1.1	8
26	Accurate CHIPR Potential Energy Surface for the Lowest Triplet State of C₃. Journal of Physical Chemistry A, 2019, 123, 8154-8169.	1.1	13
27	A trajectory surface hopping study of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si45.svg"><mml:mrow><mml:msub><mml:mrow><mml:mtext>N</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn mathvariant="normal">Î£</mml:mi></mml:mrow><mml:mrow><mml:mi>u</mml:mi></mml:mrow><mml:mrow><mml:mo>+</mml:mo> Chemical Physics Letters, 2019, 729, 61-64.	1.2	6
28	Optimal basis sets for CBS extrapolation of the correlation energy: oV x Z and oV(x+d)Z. Journal of Chemical Physics, 2019, 150, 154106.	1.2	2
29	CBS extrapolation of Hartreeâ€“Fock energy: Pople and Dunning basis sets hand-to-hand on the endeavour. Physical Chemistry Chemical Physics, 2019, 21, 8022-8034.	1.3	15
30	A global CHIPR potential energy surface for ground-state C₃H and exploratory dynamics studies of reaction C₂+ CH â†’ C₃+ H. Physical Chemistry Chemical Physics, 2019, 21, 24406-24418.	1.3	11
31	Difficulties and Virtues in Assessing the Potential Energy Surfaces of Carbon Clusters via DMBE Theory: Stationary Points of C_{Î½} (Î½ = 2â€“10) at the Focal Point. Journal of Physical Chemistry A, 2019, 123, 3121-3130.	1.1	5
32	Energy-switching potential energy surface for ground-state <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mtext>C</mml:mtext></mml:mrow><mml:mrow><mml:mn>3</mml:m Chemical Physics Letters, 2018, 700, 36-43.	1.2	9
33	Accurate Explicit-Correlation-MRCI-Based DMBE Potential-Energy Surface for Ground-State CNO. Journal of Physical Chemistry A, 2018, 122, 4198-4207.	1.1	13
34	C _n (n =2â˜4): current status. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2018, 376, 20170145.	1.6	21
35	Straightening the Hierarchical Staircase for Basis Set Extrapolations: A Low-Cost Approach to High-Accuracy Computational Chemistry. Annual Review of Physical Chemistry, 2018, 69, 177-203.	4.8	65
36	Accurate ab initio potential for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si9.gif" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>HO</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</m CBS extrapolated energies and direct-fit diatomic curves. Chemical Physics Letters, 2018, 691, 421-430.	1.2	7

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37	Multiple conical intersections in small linear parameter Jahnâ€“Teller systems: the DMBE potential energy surface of ground-state C₃ revisited. Physical Chemistry Chemical Physics, 2018, 20, 10319-10331.	1.3	6
38	3D time-dependent wave-packet approach in hyperspherical coordinates for the H + O₂ reaction on the CHIPR and DMBE IV potential energy surfaces. Physical Chemistry Chemical Physics, 2018, 20, 478-488.	1.3	17
39	The O + NO(v) Vibrational Relaxation Processes Revisited. Journal of Physical Chemistry A, 2018, 122, 5299-5310.	1.1	10
40	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.	1.3	25
41	Even numbered carbon clusters: cost-effective wavefunction-based method for calculation and automated location of most structural isomers. European Physical Journal D, 2018, 72, 1.	0.6	11
42	Assessing How Correlated Molecular Orbital Calculations Can Perform versus Kohnâ€“Sham DFT: Barrier Heights/Isomerizations. Chemistry - A European Journal, 2017, 23, 9122-9129.	1.7	14
43	Coupled 3D time-dependent quantum wave-packet study of the O + OH reaction in hyperspherical coordinates on the CHIPR potential energy surface. Chemical Physics Letters, 2017, 675, 85-91.	1.2	11
44	The Jahn-Teller plus pseudo-Jahn-Teller vibronic problem in the C3 radical and its topological implications. Journal of Chemical Physics, 2016, 144, 064309.	1.2	19
45	Role of (H₂O)_n (n = 2â€“3) Clusters on the HO₂ + O₃ Reaction: A Theoretical Study. Journal of Physical Chemistry B, 2016, 120, 1560-1568.	1.2	26
46	Sub-femtosecond nuclear dynamics and high-harmonic generation: Can muonated species be used as a probe of isotope effects?. Chemical Physics Letters, 2016, 653, 47-53.	1.2	2
47	Modeling cusps in adiabatic potential energy surfaces using a generalized Jahn-Teller coordinate. Chemical Physics Letters, 2016, 660, 55-59.	1.2	12
48	Carbon Dioxide Capture and Release by Anions with Solventâ€Dependent Behaviour: A Theoretical Study. Chemistry - A European Journal, 2016, 22, 14056-14063.	1.7	12
49	Similarity measures between excited singlet and triplet electron densities in linear acenes: an application to singlet fission. Molecular Physics, 2016, 114, 3650-3657.	0.8	1
50	Extrapolation of Hartreeâ€“Fock and multiconfiguration self-consistent-field energies to the complete basis set limit. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	28
51	The HO2 + (H2O)n + O3 reaction: an overview and recent developments. European Physical Journal D, 2016, 70, 1.	0.6	11
52	Structural evolution of the methane cation in subfemtosecond photodynamics. Journal of Chemical Physics, 2015, 143, 014304.	1.2	17
53	Rescattering of recolliding electron and low energy structure in few-cycle mid-infrared strong laser field: A 3D-TDSE study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2015, 379, 1133-1138.	0.9	0
54	On dipositronium and molecular hydrogen: similarities and differences. European Physical Journal D, 2015, 69, 1.	0.6	4

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55	Coupled 3D Time-Dependent Wave-Packet Approach in Hyperspherical Coordinates: The D⁺+H₂ Reaction on the Triple-Sheeted DMBE Potential Energy Surface. Journal of Physical Chemistry A, 2015, 119, 12392-12403.	1.1	26
56	Mapping the HO3 ground state potential energy surface with DFT: Can we reproduce the MRCI+Q/CBS data?. Chemical Physics Letters, 2015, 620, 61-66.	1.2	4
57	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.	1.1	14
58	Modeling Cusps in Adiabatic Potential Energy Surfaces. Journal of Physical Chemistry A, 2015, 119, 1415-1421.	1.1	15
59	Quantum dynamics study on the CHIPR potential energy surface for the hydroperoxyl radical: The reactions O + OHâ‡O2 + H. Journal of Chemical Physics, 2015, 142, 014309.	1.2	13
60	Subfemtosecond Quantum Nuclear Dynamics in Water Isotopomers. Journal of Physical Chemistry A, 2015, 119, 4856-4863.	1.1	7
61	Sub-femtosecond quantum dynamics of the strong-field ionization of water to the XÌƒ²B₁ and Ãƒ²A₁ states of the cation. Physical Chemistry Chemical Physics, 2015, 17, 6545-6553.	1.3	8
62	Accurate adiabatic potential energy surface for 12Aâ€² state of FH2 based on ab initio data extrapolated to the complete basis set limit. European Physical Journal D, 2015, 69, 1.	0.6	8
63	Toward a unified single-parameter extrapolation scheme for the correlation energy: Systems formed by atoms of hydrogen through neon. Chemical Physics Letters, 2015, 631-632, 70-77.	1.2	24
64	Effect of Initial Vibrational-State Excitation on Subfemtosecond Photodynamics of Water. Journal of Physical Chemistry A, 2015, 119, 12367-12375.	1.1	4
65	Low-temperature D+ + H2 reaction: A time-dependent coupled wave-packet study in hyperspherical coordinates. Journal of Chemical Physics, 2015, 142, 024304.	1.2	27
66	Accurate ab initio-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.	1.2	19
67	Quantum dynamics study of the X+O2 reactions on the CHIPR potential energy surface: X=Mu, H, D, T. Chemical Physics Letters, 2015, 638, 61-65.	1.2	6
68	On the performance of various hierarchized bases in extrapolating the correlation energy to the complete basis set limit. Chemical Physics Letters, 2015, 641, 90-96.	1.2	27
69	Dynamics of the O + ClO Reaction: Reactive and Vibrational Relaxation Processes. Journal of Physical Chemistry A, 2014, 118, 12120-12129.	1.1	1
70	Carbon Dioxide Capture with the Ozone-like Polynitrogen Molecule Li₃N₃. Journal of Physical Chemistry A, 2014, 118, 12256-12261.	1.1	5
71	Coupledâ€cluster reaction barriers of : An application of the coupledâ€cluster//Kohnâ€“Sham density functional theory model chemistry. Journal of Computational Chemistry, 2014, 35, 507-517.	1.5	20
72	Oddâ€hydrogen: An account on electronic structure, kinetics, and role of water in mediating reactions with atmospheric ozone. Just a catalyst or far beyond?. International Journal of Quantum Chemistry, 2014, 114, 1327-1349.	1.0	21

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73	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.	1.2	76
74	Accurate double many-body expansion potential energy surface for the 21Aâ€² state of N2O. Journal of Chemical Physics, 2014, 141, 084307.	1.2	11
75	On the ferryl catalyst: Electronic structure and optimized ab initio geometry. Chemical Physics Letters, 2014, 595-596, 175-179.	1.2	5
76	Quasiclassical Trajectory Study of the Atmospheric Reaction N(²D) + NO(X) Tj ETQq0 0 0 rgBT /Overlock 10	1.1	18
77	On carbon dioxide capture: An accurate ab initio study of the Li3N+CO2 insertion reaction. Computational and Theoretical Chemistry, 2014, 1036, 61-71.	1.1	6
78	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.	1.1	6
79	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.	1.3	5
80	Theoretical investigation of vibrational relaxation of highly excited O3 in collisions with HO2. RSC Advances, 2014, 4, 9866.	1.7	1
81	On Extracting Subfemtosecond Data from Femtosecond Quantum Dynamics Calculations: The Methane Cation. Journal of Chemical Theory and Computation, 2014, 10, 3606-3616.	2.3	20
82	Electronic Quenching in N(²D) + N₂ Collisions: A State-Specific Analysis via Surface Hopping Dynamics. Journal of Chemical Theory and Computation, 2014, 10, 1872-1877.	2.3	16
83	Coupled 3D Time-Dependent Wave-Packet Approach in Hyperspherical Coordinates: Application to the Adiabatic Singlet-State(1¹Aâ€²) D⁺ + H₂ Reaction. Journal of Physical Chemistry A, 2014, 118, 4837-4850.	1.1	26
84	Orbitals of the dipositronium. Chemical Physics Letters, 2014, 610-611, 167-172.	1.2	4
85	Photoinduced coupled twisted intramolecular charge transfer and excited-state proton transfer via intermolecular hydrogen bonding: A DFT/TD-DFT study. Chemical Physics Letters, 2014, 610-611, 179-185.	1.2	8
86	Single-Sheeted Double Many-Body Expansion Potential Energy Surface for Ground-State ClO₂. Journal of Physical Chemistry A, 2014, 118, 4851-4862.	1.1	6
87	Benchmarking of Density Functionals for the Accurate Description of Thiolâ€“Disulfide Exchange. Journal of Chemical Theory and Computation, 2014, 10, 4842-4856.	2.3	33
88	Roadmap to spline-fitting potentials in high dimensions. Journal of Mathematical Chemistry, 2013, 51, 1729-1746.	0.7	15
89	Vibrational energy transfer in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si20.gif" overflow="scroll"><mml:mrow><mml:mi mathvariant="normal">N</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:msup><mml:mrow) Tj ETQq1 1 0.784314 rgBT /Ove	1.2	9
90	Silane Radical Cation: A Theoretical Account on the Jahnâ€“Teller Effect at a Triple Degeneracy. Journal of Physical Chemistry A, 2013, 117, 8794-8805.	1.1	3

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91	Accurate Determination of the Reaction Course in HY₂ â‡Œ Y + YH (Y = O, S): Detailed Analysis of the Covalent- to Hydrogen-Bonding Transition. Journal of Physical Chemistry A, 2013, 117, 7393-7407.	1.1	16
92	Combined-hyperbolic-inverse-power-representation of potential energy surfaces: A preliminary assessment for H3 and HO2. Journal of Chemical Physics, 2013, 138, 054120.	1.2	36
93	Accurate Study of the Two Lowest Singlet States of HN₃: Stationary Structures and Energetics at the MRCI Complete Basis Set Limit. Journal of Physical Chemistry A, 2013, 117, 4044-4050.	1.1	7
94	Electronic Quenching of N(²D) by N₂: Theoretical Predictions, Comparison with Experimental Rate Constants, and Impact on Atmospheric Modeling. Journal of Physical Chemistry Letters, 2013, 4, 2292-2297.	2.1	22
95	The coupled 3D wave packet approach for triatomic reactive scattering in hyperspherical coordinates. Computer Physics Communications, 2013, 184, 270-283.	3.0	35
96	Accurate combined-hyperbolic-inverse-power-representation of ab initio potential energy surface for the hydroperoxyl radical and dynamics study of $f O+OH$O+OH reaction. Journal of Chemical Physics, 2013, 138, 134117.	1.2	36
97	Manifestation of external field effect in time-resolved photo-dissociation dynamics of LiF. Chinese Physics B, 2013, 22, 073303.	0.7	2
98	Implications of the O + OH reaction in hydroxyl nightglow modeling. Atmospheric Chemistry and Physics, 2013, 13, 1-13.	1.9	60
99	Accurate Potential Energy Surfaces and Beyond: Chemical Reactivity, Binding, Long-Range Interactions, and Spectroscopy. Advances in Physical Chemistry, 2012, 2012, 1-4.	2.0	9
100	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.	1.2	12
101	A detailed test study of barrier heights for the HO2 + H2O + O3 reaction with various forms of multireference perturbation theory. Journal of Chemical Physics, 2012, 136, 114312.	1.2	10
102	Accurate ab-Initio-Based Single-Sheeted DMBE Potential-Energy Surface for Ground-State N₂O. Journal of Physical Chemistry A, 2012, 116, 4646-4656.	1.1	19
103	N(4Sâ€‰/2D)+N2: Accurate ab initio-based DMBE potential energy surfaces and surface-hopping dynamics. Journal of Chemical Physics, 2012, 137, 22A515.	1.2	27
104	Ab Initio Treatment of Bond-Breaking Reactions: Accurate Course of HO₃ Dissociation and Revisit to Isomerization. Journal of Chemical Theory and Computation, 2012, 8, 428-441.	2.3	45
105	Ab Initio-Based Global Double Many-Body Expansion Potential Energy Surface for the First 2Aâ€³ Electronic State of NO2. Journal of Physical Chemistry A, 2012, 116, 3023-3034.	1.1	17
106	Accurate ab initioâ€based double manyâ€body expansion adiabatic potential energy surface for the 2² A^{â€²} state of NH₂ by extrapolation to the complete basis set limit. International Journal of Quantum Chemistry, 2012, 112, 2932-2939.	1.0	13
107	Dynamics study of a three-fold pseudo-Jahnâ€“Teller system using the extended Longuetâ€“Higgins formalism. Journal of Chemical Sciences, 2012, 124, 115-120.	0.7	0
108	Can water be a catalyst on the HO2+H2O+O3 reactive cluster?. Chemical Physics, 2012, 399, 17-22.	0.9	19

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109	An accurate ab initio potential energy curve and the vibrational bound states of state of. Chemical Physics, 2012, 398, 160-167.	0.9	10
110	Toward the modeling of the NO₂(²A^{â€³}) manifold. International Journal of Quantum Chemistry, 2011, 111, 3776-3785.	1.0	12
111	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.	1.3	26
112	Is HO3 minimum cis or trans? An analytic full-dimensional ab initio isomerization path. Physical Chemistry Chemical Physics, 2011, 13, 9796.	1.3	35
113	Accurate Double Many-Body Expansion Potential Energy Surface for Ground-State HS₂Based on ab Initio Data Extrapolated to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2011, 115, 5274-5283.	1.1	30
114	Quasiclassical Trajectory Study of the C(¹D) + H₂ Reaction and Isotopomeric Variants: Kinetic Isotope Effect and CD/CH Branching Ratio. Journal of Physical Chemistry A, 2011, 115, 7882-7890.	1.1	25
115	Ab Initio Based Double-Sheeted DMBE Potential Energy Surface for N₃(²Aâ€³) and Exploratory Dynamics Calculations. Journal of Physical Chemistry A, 2011, 115, 12390-12398.	1.1	26
116	Generalized Bornâ€“Oppenheimer treatment of Jahnâ€“Teller systems in Hilbert spaces of arbitrary dimension: theory and application to a three-state model potential. Physical Chemistry Chemical Physics, 2011, 13, 8131.	1.3	13
117	On the stability of the elusive HO3 radical. Physical Chemistry Chemical Physics, 2011, 13, 15619.	1.3	37
118	The Jahn-Teller effect in the triply degenerate electronic state of methane radical cation. Journal of Chemical Physics, 2011, 135, 174304.	1.2	24
119	18th European Conference on Dynamics of Molecular Systems. Physica Scripta, 2011, 84, 028101.	1.2	0
120	Significant nonadiabatic effects in the C + CH reaction dynamics. Journal of Chemical Physics, 2011, 135, 024306.	1.2	13
121	Refining to near spectroscopic accuracy the double many-body expansion potential energy surface for ground-state NH2. Chemical Physics Letters, 2011, 516, 17-22.	1.2	14
122	A study of the geometrical phase effect on scattering processes: Validity of the extended-Longuetâ€“Higgins formalism for a four-fold Jahnâ€“Teller type model system. Chemical Physics, 2011, 389, 81-87.	0.9	3
123	Heliumâ€fullerene pair interactions: An ab initio study by perturbation theory and coupled cluster methods. International Journal of Quantum Chemistry, 2011, 111, 416-429.	1.0	14
124	Quasiclassical trajectory study of the rotational distribution for the O+NO(v = 0) fundamental vibrational excitation. International Journal of Chemical Kinetics, 2011, 43, 345-352.	1.0	3
125	The reaction: Current status and prospective work. Computational and Theoretical Chemistry, 2011, 965, 291-297.	1.1	15
126	Quantum calculations for the S(1D)+H2reaction employing the ground adiabatic electronic state. Physica Scripta, 2011, 84, 028102.	1.2	14

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127	On the role of dynamical barriers in barrierless reactions at low energies: S(1D) + H2. Journal of Chemical Physics, 2011, 135, 134313.	1.2	26
128	Geometrical phase effect in Jahnâ€“Teller systems: Twofold electronic degeneracies and beyond. Chemical Physics Letters, 2010, 487, 139-146.	1.2	22
129	Quasi-classical trajectory and quantum mechanics study of the reaction H(2S)+NHâ†'N(4S)+H2. Chemical Physics Letters, 2010, 493, 225-228.	1.2	39
130	Adiabatic quantum dynamics calculations of the rate constant for the N+NHâ†'N2+H reaction. Chemical Physics Letters, 2010, 497, 159-162.	1.2	6
131	Spin-component-scaling second-order MÃ¸llerâ€“Plesset theory and its variants for economical correlation energies: Unified theoretical interpretation and use for quartet N3. Journal of Chemical Physics, 2010, 133, 064104.	1.2	16
132	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.	1.1	69
133	Ab Initio Study of Hydrazinyl Radical: Toward a DMBE Potential Energy Surface. Journal of Physical Chemistry A, 2010, 114, 11663-11669.	1.1	3
134	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.	1.1	28
135	Accurate MRCI and CC Study of the Most Relevant Stationary Points and Other Topographical Attributes for the Ground-State C₂H₂ Potential Energy Surface. Journal of Physical Chemistry A, 2010, 114, 13277-13287.	1.1	24
136	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.	1.1	22
137	HO₂ + O₃ Reaction: Ab Initio Study and Implications in Atmospheric Chemistry. Journal of Chemical Theory and Computation, 2010, 6, 412-420.	2.3	20
138	How Well Can Kohnâ^'Sham DFT Describe the HO₂ + O₃ Reaction?. Journal of Chemical Theory and Computation, 2010, 6, 2751-2761.	2.3	21
139	Accurate Potential Energy Surface for the 1²Aâ€² State of NH₂: Scaling of External Correlation Versus Extrapolation to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2010, 114, 9644-9654.	1.1	29
140	Nonadiabatic quantum dynamics calculations for the N + NH â†' N2 + H reaction. Physical Chemistry Chemical Physics, 2010, 12, 9619.	1.3	12
141	Dynamics study of the atmospheric reaction involving vibrationally excited O3 with OH. Physical Chemistry Chemical Physics, 2010, 12, 11362.	1.3	3
142	Ab initio Based DMBE Potential Energy Surface for the Ground Electronic State of the C₂H Molecule. Journal of Physical Chemistry A, 2010, 114, 2655-2664.	1.1	7
143	Accurate Double Many-Body Expansion Potential Energy Surface for N₃(⁴Aâ€²â€²) from Correlation Scaled ab Initio Energies with Extrapolation to the Complete Basis Set Limit. Journal of Physical Chemistry A, 2009, 113, 14424-14430.	1.1	51
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