# GÃ¡bor CzakÃ³

List of Publications by Year
in descending order



| | | | |
|---|---|---|---|
| 110 papers | 4,729 citations | 81839 39 h-index | 106281 65 g-index |
| 110 all docs | 110 docs citations | 110 times ranked | 1892 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | High-dimensional ab initio potential energy surfaces for reaction dynamics calculations. Physical Chemistry Chemical Physics, 2011, 13, 8094. | 1.3 | 252 |
| 2 | The fourth age of quantum chemistry: molecules in motion. Physical Chemistry Chemical Physics, 2012, 14, 1085-1106. | 1.3 | 196 |
| 3 | Quasiclassical trajectory calculations of correlated product distributions for the F+CHD3(v1=,1) reactions using an ab initio potential energy surface. Journal of Chemical Physics, 2009, 131, 244302. | 1.2 | 190 |
| 4 | Toward black-box-type full- and reduced-dimensional variational (ro)vibrational computations. Journal of Chemical Physics, 2009, 130, 134112. | 1.2 | 180 |
| 5 | Dynamics of the Reaction of Methane with Chlorine Atom on an Accurate Potential Energy Surface. Science, 2011, 334, 343-346. | 6.0 | 167 |
| 6 | On equilibrium structures of the water molecule. Journal of Chemical Physics, 2005, 122, 214305. | 1.2 | 157 |
| 7 | Revealing a double-inversion mechanism for the Fâ¯'+CH3Cl SN2 reaction. Nature Communications, 2015, 6, 5972. | 5.8 | 134 |
| 8 | Accurate ab initio potential energy surface, dynamics, and thermochemistry of the F+CH4â†'HF+CH3 reaction. Journal of Chemical Physics, 2009, 130, 084301. | 1.2 | 130 |
| 9 | Influence of the leaving group on the dynamics of a gas-phase SN2 reaction. Nature Chemistry, 2016, 8, 151-156. | 6.6 | 116 |
| 10 | CH Stretching Excitation Steers the F Atom to the CD Bond in the F + CHD<sub>3</sub> Reaction. Journal of the American Chemical Society, 2009, 131, 17534-17535. | 6.6 | 108 |
| 11 | Theoretical Study of the Validity of the Polanyi Rules for the Late-Barrier Cl + CHD<sub>3</sub> Reaction. Journal of Physical Chemistry Letters, 2012, 3, 3416-3419. | 2.1 | 106 |
| 12 | Ab-Initio-Based Potential Energy Surfaces for Complex Molecules and Molecular Complexes. Journal of Physical Chemistry Letters, 2010, 1, 1866-1874. | 2.1 | 97 |
| 13 | Reaction Dynamics of Methane with F, O, Cl, and Br on ab Initio Potential Energy Surfaces. Journal of Physical Chemistry A, 2014, 118, 2839-2864. | 1.1 | 96 |
| 14 | Vibrational energy levels with arbitrary potentials using the Eckart-Watson Hamiltonians and the discrete variable representation. Journal of Chemical Physics, 2007, 127, 084102. | 1.2 | 90 |
| 15 | Experimental and Theoretical Investigations of Energy Transfer and Hydrogen-Bond Breaking in the Water Dimer. Journal of the American Chemical Society, 2012, 134, 15430-15435. | 6.6 | 89 |
| 16 | Mode Selectivity for a â€œCentralâ€•Barrier Reaction: Eight-Dimensional Quantum Studies of the O(<sup>3</sup>P) + CH<sub>4</sub> â†' OH + CH<sub>3</sub> Reaction on an Ab Initio Potential Energy Surface. Journal of Physical Chemistry Letters, 2012, 3, 3776-3780. | 2.1 | 87 |
| 17 | Dynamics of the O(3P) + CHD3(vCH = 0,1) reactions on an accurate ab initio potential energy surface. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 7997-8001. | 3.3 | 78 |
| 18 | Accurate ab initio potential energy surface, thermochemistry, and dynamics of the Cl(2P, 2P3/2) + CH4 â†' HCl + CH3 and H + CH3Cl reactions. Journal of Chemical Physics, 2012, 136, 044307. | 1.2 | 76 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Rotational mode specificity in the Cl + CHD3 â†' HCl + CD3 reaction. Journal of Chemical Physics, 2014, 141, 074310. | 1.2 | 75 |
| 20 | A practical method to avoid zero-point leak in molecular dynamics calculations: Application to the water dimer. Journal of Chemical Physics, 2010, 132, 164103. | 1.2 | 73 |
| 21 | Dynamics of the Fâ^' + CH3Cl â†' Clâ^' + CH3F SN2 reaction on a chemically accurate potential energy surface. Chemical Science, 2013, 4, 4362. | 3.7 | 70 |
| 22 | Variational vibrational calculations using high-order anharmonic force fields. Molecular Physics, 2004, 102, 2411-2423. | 0.8 | 65 |
| 23 | Mode-Specific S<sub>N</sub>2 Reaction Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 3322-3327. | 2.1 | 63 |
| 24 | Assigning quantum labels to variationally computed rotational-vibrational eigenstates of polyatomic molecules. Journal of Chemical Physics, 2010, 133, 034113. | 1.2 | 61 |
| 25 | Automating the Development of High-Dimensional Reactive Potential Energy Surfaces with the <scp>robosurfer</scp> Program System. Journal of Chemical Theory and Computation, 2020, 16, 51-66. | 2.3 | 60 |
| 26 | Gaussian Binning of the Vibrational Distributions for the Cl + CH<sub>4</sub>(v<sub>4/2</sub> = 0, 1) â†' H + CH<sub>3</sub>Cl(n<sub>1</sub>n<sub>2</sub>n<sub>3</sub>n<sub>4</sub>n<sub>5</sub>n<sub>6</sub>) Reactions. Journal of Physical Chemistry A, 2012, 116, 7467-7473. | 1.1 | 55 |
| 27 | Dynamics and Novel Mechanisms of S<sub>N</sub>2 Reactions on ab Initio Analytical Potential Energy Surfaces. Journal of Physical Chemistry A, 2017, 121, 9005-9019. | 1.1 | 55 |
| 28 | Chapter 9 An Active Database Approach to Complete Rotationalâ€"Vibrational Spectra of Small Molecules. Annual Reports in Computational Chemistry, 2007, 3, 155-176. | 0.9 | 54 |
| 29 | High-level ab initio potential energy surface and dynamics of the F<sup>â^'</sup>+ CH<sub>3</sub>I S<sub>N</sub>2 and proton-transfer reactions. Chemical Science, 2017, 8, 3164-3170. | 3.7 | 53 |
| 30 | Bridging Theory with Experiment: A Benchmark Study of Thermally Averaged Structural and Effective Spectroscopic Parameters of the Water Molecule. Journal of Physical Chemistry A, 2009, 113, 11665-11678. | 1.1 | 52 |
| 31 | Double-Inversion Mechanisms of the X<sup>â€"</sup> + CH<sub>3</sub>Y [X,Y = F, Cl, Br, I] S<sub>N</sub>2 Reactions. Journal of Physical Chemistry A, 2015, 119, 3134-3140. | 1.1 | 49 |
| 32 | Deciphering Front-Side Complex Formation in S<sub>N</sub>2 Reactions via Dynamics Mapping. Journal of Physical Chemistry Letters, 2017, 8, 2917-2923. | 2.1 | 49 |
| 33 | An ab initio spinâ€"orbit-corrected potential energy surface and dynamics for the F + CH4 and F + CHD3 reactions. Physical Chemistry Chemical Physics, 2011, 13, 8306. | 1.3 | 47 |
| 34 | Communication: Experimental and theoretical investigations of the effects of the reactant bending excitations in the F+CHD3 reaction. Journal of Chemical Physics, 2010, 133, 131101. | 1.2 | 46 |
| 35 | Experimental and Theoretical Investigations of Energy Transfer and Hydrogen-Bond Breaking in Small Water and HCl Clusters. Accounts of Chemical Research, 2014, 47, 2700-2709. | 7.6 | 46 |
| 36 | Accurate ab initio determination of spectroscopic and thermochemical properties of mono- and dichlorocarbenes. Physical Chemistry Chemical Physics, 2005, 7, 2881. | 1.3 | 43 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Conformers of gaseous threonine. Molecular Physics, 2009, 107, 761-775. | 0.8 | 43 |
| 38 | Atomistic dynamics of elimination and nucleophilic substitution disentangled for the Fâ¯â€‰+â€‰CH3CH2Cl reaction. Nature Chemistry, 2021, 13, 977-981. | 6.6 | 43 |
| 39 | Anchoring the Absolute Proton Affinity Scale. Journal of Chemical Theory and Computation, 2008, 4, 1220-1229. | 2.3 | 42 |
| 40 | Quasiclassical Trajectory Studies of the O(<sup>3</sup>P) + CX<sub>4</sub>(v<sub>k</sub> = 0, 1) â†’ OX(v) + CX<sub>3</sub>(n<sub>1</sub>n<sub>2</sub>n<sub>3</sub>n<sub>4</sub>) [X = H and D] Reactions on an Ab Initio Potential Energy Surface. Journal of Physical Chemistry A, 2013, 117, 6409-6420. | 1.1 | 41 |
| 41 | On one-dimensional discrete variable representations with general basis functions. Journal of Chemical Physics, 2003, 119, 10512-10518. | 1.2 | 39 |
| 42 | Direct mapping of the angle-dependent barrier to reaction for Clâ€‰+â€‰CHD3 using polarized scattering data. Nature Chemistry, 2017, 9, 1175-1180. | 6.6 | 37 |
| 43 | Stretching vibration is a spectator in nucleophilic substitution. Science Advances, 2018, 4, eaas9544. | 4.7 | 37 |
| 44 | Accurate ab initio potential energy surface, thermochemistry, and dynamics of the Br(2P, 2P3/2) + CH4 â†’ HBr + CH3 reaction. Journal of Chemical Physics, 2013, 138, 134301. | 1.2 | 36 |
| 45 | On the Choice of the Ab Initio Level of Theory for Potential Energy Surface Developments. Journal of Physical Chemistry A, 2014, 118, 646-654. | 1.1 | 36 |
| 46 | Communication: Probing the entrance channels of the X + CH4 â†’ HX + CH3 (X = F, Cl, Br, I) reactions via photodetachment of Xâ¯â€“CH4. Journal of Chemical Physics, 2011, 134, 191102. | 1.2 | 35 |
| 47 | Rethinking the X<sup>â¯</sup> + CH<sub>3</sub>Y [X = OH, SH, CN, NH<sub>2</sub>, PH<sub>2</sub>; Y = F, Cl, Br, I] S<sub>N</sub>2 reactions. Physical Chemistry Chemical Physics, 2019, 21, 7924-7931. | 1.3 | 35 |
| 48 | Proton affinity and enthalpy of formation of formaldehyde. International Journal of Quantum Chemistry, 2009, 109, 2393-2409. | 1.0 | 33 |
| 49 | On the efficiency of treating singularities in triatomic variational vibrational computations. The vibrational states of H+3 up to dissociation. Physical Chemistry Chemical Physics, 2010, 12, 8373. | 1.3 | 33 |
| 50 | Communication: Quasiclassical trajectory calculations of correlated product-state distributions for the dissociation of (H2O)2 and (D2O)2. Journal of Chemical Physics, 2011, 135, 151102. | 1.2 | 33 |
| 51 | Accurate ab initio potential energy surface, thermochemistry, and dynamics of the Fâ¯ + CH3F SN2 and proton-abstraction reactions. Journal of Chemical Physics, 2015, 142, 244301. | 1.2 | 33 |
| 52 | Translational energy dependence of the Clâ€‰+â€‰CH4(vbâ€‰=â€‰0,â€‰1) reactions: a joint crossed-beam and quasiclassical trajectory study. Molecular Physics, 2012, 110, 1617-1626. | 0.8 | 32 |
| 53 | The methylene saga continues: Stretching fundamentals and zero-point energy of CH2. Journal of Molecular Structure, 2006, 780-781, 283-294. | 1.8 | 31 |
| 54 | Zero-point energy constrained quasiclassical, classical, and exact quantum simulations of isomerizations and radial distribution functions of the water trimer using an ab initio potential energy surface. Chemical Physics Letters, 2010, 500, 217-222. | 1.2 | 31 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | Quantum Dynamics Study of the F + CH<sub>4</sub> â†' HF + CH<sub>3</sub> Reaction on an Ab Initio Potential Energy Surface. Journal of Physical Chemistry A, 2013, 117, 7124-7130. | 1.1 | 30 |
| 56 | Theory Finally Agrees with Experiment for the Dynamics of the Cl + C<sub>2</sub>H<sub>6</sub> Reaction. Journal of Physical Chemistry Letters, 2020, 11, 4762-4767. | 2.1 | 28 |
| 57 | Benchmark ab Initio Characterization of the Inversion and Retention Pathways of the OH<sup>â€“</sup> + CH<sub>3</sub>Y [Y = F, Cl, Br, I] S<sub>N</sub>2 Reactions. Journal of Physical Chemistry A, 2018, 122, 5773-5780. | 1.1 | 26 |
| 58 | Accurate ab Initio Structure, Dissociation Energy, and Vibrational Spectroscopy of the Fâ¯â¯CH4 Anion Complex. Journal of Physical Chemistry A, 2008, 112, 7466-7472. | 1.1 | 25 |
| 59 | Benchmark ab Initio Characterization of the Complex Potential Energy Surface of the F<sup>â€“</sup> + CH<sub>3</sub>CH<sub>2</sub>Cl Reaction. Journal of Physical Chemistry A, 2017, 121, 2847-2854. | 1.1 | 25 |
| 60 | Benchmark ab Initio Characterization of the Complex Potential Energy Surface of the Cl<sup>â€“</sup> + CH<sub>3</sub>I Reaction. Journal of Physical Chemistry A, 2017, 121, 5748-5757. | 1.1 | 23 |
| 61 | Effects of the Level of Electronic Structure Theory on the Dynamics of the F<sup>â€“</sup> + CH<sub>3</sub>I Reaction. Journal of Physical Chemistry A, 2018, 122, 3353-3364. | 1.1 | 22 |
| 62 | Detailed benchmark ab initio mapping of the potential energy surfaces of the X + C2H6 [X = F, Cl, Br, I] reactions. Physical Chemistry Chemical Physics, 2019, 21, 396-408. | 1.3 | 20 |
| 63 | On the development of a gold-standard potential energy surface for the OH<sup>â¯</sup> + CH<sub>3</sub>I reaction. Physical Chemistry Chemical Physics, 2020, 22, 3775-3778. | 1.3 | 20 |
| 64 | Quasiclassical Trajectory Study of the Rotational Mode Specificity in the O(<sup>3</sup>P) + CHD<sub>3</sub>(v<sub>1</sub> = 0, 1, JK) â†' OH + CD<sub>3</sub> Reactions. Journal of Physical Chemistry A, 2014, 118, 11683-11687. | 1.1 | 17 |
| 65 | Benchmark ab initio and dynamical characterization of the stationary points of reactive atom + alkane and S<sub>N</sub>2 potential energy surfaces. Physical Chemistry Chemical Physics, 2020, 22, 4298-4312. | 1.3 | 17 |
| 66 | Full-dimensional MRCI-F12 potential energy surface and dynamics of the F(2P3/2) + C2H6 â†' HF + C2H5 reaction. Journal of Chemical Physics, 2020, 153, 064305. | 1.2 | 17 |
| 67 | Uncovering an oxide ion substitution for the OH<sup>â¯</sup> + CH<sub>3</sub>F reaction. Chemical Science, 2021, 12, 14369-14375. | 3.7 | 17 |
| 68 | Benchmark ab Initio Characterization of the Complex Potential Energy Surfaces of the X<sup>â€“</sup> + NH<sub>2</sub>Y [X, Y = F, Cl, Br, I] Reactions. Journal of Physical Chemistry A, 2018, 122, 1886-1895. | 1.1 | 16 |
| 69 | Mode-Specific Quasiclassical Dynamics of the F<sup>â€“</sup> + CH<sub>3</sub>I S<sub>N</sub>2 and Proton-Transfer Reactions. Journal of Physical Chemistry A, 2018, 122, 8143-8151. | 1.1 | 16 |
| 70 | Benchmark ab initio characterization of the abstraction and substitution pathways of the OH + CH4/C2H6 reactions. Physical Chemistry Chemical Physics, 2020, 22, 14560-14569. | 1.3 | 16 |
| 71 | Mode-specific multi-channel dynamics of the Fâ¯ + CHD2Cl reaction on a global ab initio potential energy surface. Journal of Chemical Physics, 2016, 145, 134303. | 1.2 | 15 |
| 72 | Flame Inhibition Chemistry: Rate Coefficients of the Reactions of HBr with CH<sub>3</sub> and OH Radicals at High Temperatures Determined by Quasiclassical Trajectory Calculations. Energy & Fuels, 2018, 32, 10100-10105. | 2.5 | 15 |

| # | ARTICLE | IF | CITATIONS |
|---|---|---|---|
| 73 | Treating singularities present in the Sutcliffe-Tennyson vibrational Hamiltonian in orthogonal internal coordinates. Journal of Chemical Physics, 2005, 122, 024101. | 1.2 | 14 |
| 74 | Adiabatic Jacobi corrections on the vibrational energy levels of H2+ isotopologues. Journal of Chemical Physics, 2009, 130, 134314. | 1.2 | 14 |
| 75 | Exact quantum dynamics background of dispersion interactions: case study for CH<sub>4</sub>Â·Ar in full (12) dimensions. Physical Chemistry Chemical Physics, 2020, 22, 2792-2802. | 1.3 | 14 |
| 76 | Numerical separation of the front-side attack and double-inversion retention pathways of SN2 reactions. Chemical Physics Letters, 2020, 755, 137780. | 1.2 | 14 |
| 77 | Facilitated inversion complicates the stereodynamics of an S<sub>N</sub>2 reaction at nitrogen center. Chemical Science, 2021, 12, 5410-5418. | 3.7 | 14 |
| 78 | First-Principles Reaction Dynamics beyond Six-Atom Systems. Journal of Physical Chemistry A, 2021, 125, 2385-2393. | 1.1 | 14 |
| 79 | Vibrational mode-specificity in the dynamics of the Cl + C2H6 â†' HCl + C2H5 reaction. Journal of Chemical Physics, 2021, 155, 114303. | 1.2 | 14 |
| 80 | Correlated Dynamics of the O(<sup>3</sup>P) + CHD<sub>3</sub>(v=0) Reaction: A Joint Crossed-Beam and Quasiclassical Trajectory Study. Journal of Physical Chemistry A, 2015, 119, 7190-7196. | 1.1 | 13 |
| 81 | Uncovering the role of the stationary points in the dynamics of the F<sup>â^'</sup> + CH<sub>3</sub>I reaction. Physical Chemistry Chemical Physics, 2019, 21, 1578-1586. | 1.3 | 13 |
| 82 | Conformers of dehydrogenated glycine isomers. Journal of Computational Chemistry, 2020, 41, 2001-2014. | 1.5 | 13 |
| 83 | Finite basis representations with nondirect product basis functions having structure similar to that of spherical harmonics. Journal of Chemical Physics, 2006, 124, 014110. | 1.2 | 12 |
| 84 | A paradox of grid-based representation techniques: accurate eigenvalues from inaccurate matrix elements. Journal of Mathematical Chemistry, 2012, 50, 636-651. | 0.7 | 12 |
| 85 | Vibrational mode-specific dynamics of the F<sup>â^'</sup> + CH<sub>3</sub>CH<sub>2</sub>Cl multi-channel reaction. Physical Chemistry Chemical Physics, 2022, 24, 8166-8181. | 1.3 | 12 |
| 86 | Reduced-Dimensional Quantum Computations for the Rotationalâ€"Vibrational Dynamics of F<sup>â€"</sup>CH<sub>4</sub> and F<sup>â€"</sup>CH<sub>2</sub>D<sub>2</sub>. Journal of Physical Chemistry A, 2013, 117, 6975-6983. | 1.1 | 11 |
| 87 | Communication: Direct comparison between theory and experiment for correlated angular and product-state distributions of the ground-state and stretching-excited O(3P) + CH4 reactions. Journal of Chemical Physics, 2014, 140, 231102. | 1.2 | 11 |
| 88 | ManyHF: A pragmatic automated method of finding lower-energy Hartreeâ€"Fock solutions for potential energy surface development. Journal of Chemical Physics, 2022, 156, 071101. | 1.2 | 11 |
| 89 | Does the Cl + CH<sub>4</sub> â†' H + CH<sub>3</sub>Cl Reaction Proceed via Walden Inversion?. Journal of Physical Chemistry A, 2017, 121, 9415-9420. | 1.1 | 10 |
| 90 | High-Level-Optimized Stationary Points for the F<sup>â€"</sup>(H<sub>2</sub>O) + CH<sub>3</sub>I System: Proposing a New Water-Induced Double-Inversion Pathway. Journal of Physical Chemistry A, 2019, 123, 454-462. | 1.1 | 10 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | High-Level Systematic Ab Initio Comparison of Carbon- and Silicon-Centered S<sub>N</sub>2 Reactions. Journal of Physical Chemistry A, 2021, 125, 9645-9657. | 1.1 | 10 |
| 92 | Rotational Mode Specificity in the F<sup>â€“</sup> + CH<sub>3</sub>Y [Y = F and Cl] S<sub>N</sub>2 Reactions. Journal of Physical Chemistry A, 2015, 119, 12231-12237. | 1.1 | 9 |
| 93 | Benchmark ab initio proton affinity of glycine. Physical Chemistry Chemical Physics, 2021, 23, 9663-9671. | 1.3 | 9 |
| 94 | Vibrational mode-specific dynamics of the F(2P3/2) + C2H6 â†' HF + C2H5 reaction. Journal of Chemical Physics, 2021, 155, 154302. | 1.2 | 9 |
| 95 | Use of a nondirect-product basis for treating singularities in triatomic rotationalâ€“vibrational calculations. Physical Chemistry Chemical Physics, 2007, 9, 3407. | 1.3 | 8 |
| 96 | Temperature-Dependent, Effective Structures of the <sup>14</sup>NH<sub>3</sub> and <sup>14</sup>ND<sub>3</sub> Molecules. Journal of Physical Chemistry A, 2012, 116, 4356-4362. | 1.1 | 8 |
| 97 | Benchmark ab initio stationary-point characterization of the complex potential energy surface of the multi-channel Cl + CH<sub>3</sub>NH<sub>2</sub> reaction. Physical Chemistry Chemical Physics, 2021, 23, 10347-10356. | 1.3 | 7 |
| 98 | A benchmark ab initio study of the complex potential energy surfaces of the OH<sup>â^'</sup> + CH<sub>3</sub>CH<sub>2</sub>Y [Y = F, Cl, Br, I] reactions. Physical Chemistry Chemical Physics, 2021, 23, 13526-13534. | 1.3 | 7 |
| 99 | S<sub>N</sub>2 Reactions with an Ambident Nucleophile: A Benchmark Ab Initio Study of the CN<sup>â€“</sup> + CH<sub>3</sub>Y [Y = F, Cl, Br, and I] Systems. Journal of Physical Chemistry A, 2022, 126, 889-900. | 1.1 | 7 |
| 100 | Adiabatic Jacobi corrections for H2+-like systems. Journal of Chemical Physics, 2007, 126, 024102. | 1.2 | 6 |
| 101 | Surprising Quenching of the Spinâ€“Orbit Interaction Significantly Diminishes H<sub>2</sub>OÂ·Â·X [X = F, Cl, Br, I] Dissociation Energies. Journal of Physical Chemistry A, 2014, 118, 11956-11961. | 1.1 | 6 |
| 102 | Unconventional SN2 retention pathways induced by complex formation: High-level dynamics investigation of the NH2â^' + CH3I polyatomic reaction. Journal of Chemical Physics, 2022, 156, 184306. | 1.2 | 6 |
| 103 | Pathways for the OH + Cl2 â†' HOCl + Cl and HOCl + Cl â†' HCl + ClO Reactions. Journal of Physical Chemistry A, 2015, 119, 7802-7809. | 1.1 | 5 |
| 104 | Dynamics of proton transfer from ArH+ to CO. International Journal of Mass Spectrometry, 2019, 438, 175-185. | 0.7 | 5 |
| 105 | Rotational Mode Specificity in the F<sup>â€“</sup> + CH<sub>3</sub>I(v = 0, JK) S<sub>N</sub>2 and Proton-Transfer Reactions. Journal of Physical Chemistry A, 2020, 124, 8943-8948. | 1.1 | 5 |
| 106 | Detailed quasiclassical dynamics of the Fâ^' + CH3Br reaction on an ab initio analytical potential energy surface. Journal of Chemical Physics, 2021, 155, 124301. | 1.2 | 5 |
| 107 | Benchmark ab initio proton affinity and gasâ€phase basicity of Î±â€alanine based on coupledâ€cluster theory and statistical mechanics. Journal of Computational Chemistry, 2022, 43, 19-28. | 1.5 | 4 |
| 108 | Rotational Mode-Specificity in the Cl + C<sub>2</sub>H<sub>6</sub> â†' HCl + C<sub>2</sub>H<sub>5</sub> Reaction. Journal of Physical Chemistry A, 2022, 126, 2551-2560. | 1.1 | 4 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | Benchmark Ab Initio Characterization of the Abstraction and Substitution Pathways of the Cl + CH<sub>3</sub>CN Reaction. Journal of Physical Chemistry A, 2022, 126, 2802-2810. | 1.1 | 2 |
| 110 | Conformers of gaseous threonine. , 0, . | | 1 |