

Estimation, Computation, and Experimental Correction Vibrational Energies

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Assessing a new nonempirical density functional: Difficulties in treating π -conjugation effects. Journal of Chemical Physics, 2006, 124, 124112.	1.2	34
2	One-Dimensional Free-Energy Profiles of Complex Systems: \hat{A} Progress Variables that Preserve the Barriers. Journal of Physical Chemistry B, 2006, 110, 12689-12698.	1.2	105
3	Surface-Mediated Nucleation in the Solid-State Polymorph Transformation of Terephthalic Acid. Journal of the American Chemical Society, 2007, 129, 4714-4723.	6.6	83
4	Experimental Vibrational Zero-Point Energies: Diatomic Molecules. Journal of Physical and Chemical Reference Data, 2007, 36, 389-397.	1.9	336
5	An Evaluation of Harmonic Vibrational Frequency Scale Factors. Journal of Physical Chemistry A, 2007, 111, 11683-11700.	1.1	2,264
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7	Coarse Master Equations for Peptide Folding Dynamics. Journal of Physical Chemistry B, 2008, 112, 6057-6069.	1.2	444
8	Uncertainties in scaling factors for <i>ab initio</i> vibrational zero-point energies. Journal of Chemical Physics, 2009, 130, 114102.	1.2	74
9	Performance of Density Functional Theory for 3d Transition Metal-Containing Complexes: Utilization of the Correlation Consistent Basis Sets. Journal of Physical Chemistry A, 2009, 113, 8607-8614.	1.1	84
10	Method and basis set dependence of anharmonic ground state nuclear wave functions and zero-point energies: Application to SSSH. Journal of Chemical Physics, 2010, 132, 054105.	1.2	8
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14	Geometries and Vibrational Frequencies of Small Radicals: Performance of Coupled Cluster and More Approximate Methods. Journal of Chemical Theory and Computation, 2012, 8, 2165-2179.	2.3	42
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16	Computing UV/vis spectra from the adiabatic and vertical Franck-Condon schemes with the use of Cartesian and internal coordinates. Journal of Chemical Physics, 2013, 139, 234108.	1.2	40
17	Bromination and Accompanying Rearrangement of the Polycyclic Oxetane 2,4-Oxytwistane. Journal of Organic Chemistry, 2014, 79, 8786-8799.	1.7	8
18	Heats of formation of the amino acids re-examined by means of W1-F12 and W2-F12 theories. Theoretical Chemistry Accounts, 2014, 133, 1.	0.5	74

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19	A Theoretical Study on the Functionalisation Process of C ₁₈ Fullerene Through its Open [5,5] Cycloaddition with 4-Pyridine Nitrile Oxide. Progress in Reaction Kinetics and Mechanism, 2015, 40, 169-176.	1.1	8
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21	A simple way to predict vibrational zero point energy of organophosphorus (III) compounds. Computational and Theoretical Chemistry, 2015, 1068, 13-20.	1.1	5
22	Intermolecular Reactions of a Foiled Carbene with Carbonyl Compounds: The Effects of Trishomocyclopropyl Stabilization. Journal of Organic Chemistry, 2015, 80, 11877-11887.	1.7	4
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25	A computational chemist's guide to accurate thermochemistry for organic molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 292-310.	6.2	185
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29	Rational computing of energy levels for organic electronics: the case of 2-benzylidene-1,3-indandiones. RSC Advances, 2016, 6, 85242-85253.	1.7	2
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35	Scaling Procedures in Vibrational Spectroscopy. Challenges and Advances in Computational Chemistry and Physics, 2019, , 49-95.	0.6	3
36	Can Small Polyaromatics Describe Their Larger Counterparts for Local Reactions? A Computational Study on the H-Abstraction Reaction by an H-Atom from Polyaromatics. Journal of Physical Chemistry A, 2020, 124, 9626-9637.	1.1	8

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38	Tricyclo[2.1.0.0 ^{2,5}]pent-3-ylidene: Stereoelectronic Control of Bridge-Flapping within a Nonclassical Nucleophilic Carbene. <i>Journal of Organic Chemistry</i> , 2021, 86, 878-891.	1.7	2
39	Experimental and computational insights into the synthesis and characterization of a novel Schiff base ligand 2, 2'-[(1z, 14e)-2, 5, 8,11,14-pentaazapentadeca-1, 14-diene-diyl] diphenol. <i>CSI Transactions on ICT</i> , 2021, 9, 71-81.		0
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41	An automatized workflow from molecular dynamic simulation to quantum chemical methods to identify elementary reactions and compute reaction constants. <i>Journal of Computational Chemistry</i> , 2021, 42, 2264-2282.	1.5	6
42	First-principles study of hydrogen-vacancy interactions in CoCrFeMnNi high-entropy alloy. <i>Journal of Alloys and Compounds</i> , 2022, 922, 166259.	2.8	7
43	Carbene Routes to Cyclopropatetrahydrane. <i>Journal of Organic Chemistry</i> , 2022, 87, 16902-16906.	1.7	0
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