

Harmonic Vibrational Frequencies: An Evaluation of Quadratic Configuration Interaction, Density Functional Factors

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Citation Report

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25	Relative Stabilities and Hydride Affinities of Silatropylium and Silabenzyl Cations and Their Isomers. Comparison with the Carbon Analogues Tropylium and Benzyl Cations. Journal of the American Chemical Society, 1996, 118, 10561-10570.	13.7	38
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28	Spectroscopic studies of the $\text{B}^1\Sigma^+ - \text{X}^1\Sigma^+$ system of the jet-cooled vinoxy radical. Journal of Chemical Physics, 1997, 106, 10048-10065.	3.0	56
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4107	Infrared spectroscopy of Sc ⁺ (H ₂ O) and Sc ₂ ⁺ (H ₂ O) via argon complex predissociation: The charge dependence of cation hydration. <i>Journal of Chemical Physics</i> , 2011, 134, 014302.	3.0	36
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4216	Dynamics and Thermodynamics of Crystalline Polymorphs: β -Glycine, Analysis of Variable-Temperature Atomic Displacement Parameters. <i>Journal of Physical Chemistry A</i> , 2012, 116, 8092-8099.	2.5	24
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4226	Solid state simulation of tetramer form of 5-aminoorotic acid: The vibrational spectra and molecular structure study by using MP2 and DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 97, 948-962.	3.9	11
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4228	6-Phenyl-3-(4-pyridyl)-1,2,4-triazolo-[3,4-b][1,3,4]thiadiazole: Synthesis, experimental, theoretical characterization and biological activities. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 97, 606-615.	3.9	15
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4487	NBO, NMR, UV, FT-IR, FT-Raman spectra and molecular structure (monomeric and dimeric structures) investigation of 4-Chloro-3,5-Xylenol: A combined experimental and theoretical study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 116, 170-182.	3.9	7
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4489	Molecular structure of tetraaqua adenosine 5'-triphosphate aluminium(III) complex: A study involving Raman spectroscopy, theoretical DFT and potentiometry. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 105, 88-101.	3.9	11
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4494	Nitro \rightleftharpoons aci-nitro tautomerism and E/Z isomeric preferences of nitroethenediamine derivatives: a quantum chemical study. <i>RSC Advances</i> , 2013, 3, 25268.	3.6	12

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4507	Analysis of heat-treated graphite oxide by X-ray photoelectron spectroscopy. <i>Journal of Materials Science</i> , 2013, 48, 8171-8198.	3.7	147
4508	Molecular structure and vibrational spectral investigation of charge transfer NLO crystal Naphthalene Picrate for THz application. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 108, 256-267.	3.9	19
4509	Selected hydroxycoumarins as antioxidants in cells: physicochemical and reactive oxygen species scavenging studies. <i>Journal of Physical Organic Chemistry</i> , 2013, 26, 773-783.	1.9	14
4510	A theoretical study on 1,5-diazido-3-nitrazapentane (DANP) and 1,7-diazido-2,4,6-trinitrazaheptane (DATNH): molecular and crystal structures, thermodynamic and detonation properties, and pyrolysis mechanism. <i>Journal of Molecular Modeling</i> , 2013, 19, 5367-5376.	1.8	16
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4519	Calculation of Vibrational Spectra of p-Ethylbenzenesulfonic Acid Hydrates. <i>Journal of Applied Spectroscopy</i> , 2013, 80, 499-504.	0.7	0
4520	Analysis of Vibrational Spectra of Pyridoxazinone Based on Density Functional Theory Calculations. <i>Journal of Applied Spectroscopy</i> , 2013, 80, 492-498.	0.7	11
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4566	4-Hydroxy-2,5-dimethylphenyl-benzophenone: Conformational stability, FT-IR and Raman investigation. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 102, 386-392.	3.9	10

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4595	Structure-Making Ability of Na ⁺ in Dilute Aqueous Solution: An ONIOM-XS MD Simulation Study. <i>Journal of Physical Chemistry A</i> , 2013, 117, 1826-1833.	2.5	28
4596	New diethoxo-bridged dinuclear Cr(III) complexes with derivatives of the quinoxaline-2,3-dione ligand and 2,2'-bipyridine as a co-ligand: Syntheses, spectral characterizations, magnetic properties, antimicrobial inhibitory activities and interpretation of the electronic absorption spectra using the ZINDO/S-CI semi-empirical method. <i>Polyhedron</i> , 2013, 51, 243-254.	2.2	9
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4608	Toward a Physically Based Quantitative Modeling of Impact Sensitivities. Journal of Physical Chemistry A, 2013, 117, 2253-2259.	2.5	42
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5008	Crystal structure, DFT and HF calculations and radical scavenging activities of (E)-4,6-dibromo-3-methoxy-2-[(3-methoxyphenylimino)methyl]phenol. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 125, 319-327.	3.9	10
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5261	Syntheses, structural elucidation, thermal properties, theoretical quantum chemical studies (DFT) and biological studies of barbituricâ€“hydrazone complexes. <i>Journal of Saudi Chemical Society</i> , 2015, 19, 217-226.	5.2	14
5262	N-bromosuccinimide (NBS)-promoted, three-component synthesis of 1,2-unsaturated isoxazol-5(4H)-ones, and spectroscopic investigation and computational study of 3-methyl-4-(thiophen-2-ylmethylene)isoxazol-5(4H)-one. <i>Research on Chemical Intermediates</i> , 2015, 41, 7739-7773.	2.7	47
5263	Bimetallic zinc complex â€“ active species in coupling of terminal alkynes with aldehydes via nucleophilic addition/Oppenauer oxidation. <i>Chemical Communications</i> , 2015, 51, 576-579.	4.1	39
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