

Combination of theoretical ab initio and experimental infrared
harmonic force constants. Scaled quantum mechanical calculations for
acrolein, butadiene, formaldehyde, and ethylene

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Citation Report

#	ARTICLE	IF	CITATIONS
2	A theoretical study of the structure and vibrational spectrum of trifluoromethylperoxy radical. <i>Molecular Physics</i> , 1984, 53, 1131-1144.	0.8	7
3	Ab initio studies on hydrogen-bonded chains. IV. Structure and stability of formic acid chains. <i>Chemical Physics</i> , 1984, 88, 415-423.	0.9	26
4	Ab initio studies of structural features not easily amenable to experiment. <i>Computational and Theoretical Chemistry</i> , 1984, 109, 321-330.	1.5	29
5	Structure, complete harmonic force field, vibrational spectra and infrared intensities of triprismane (tetracyclohexane). <i>Computational and Theoretical Chemistry</i> , 1984, 109, 127-136.	1.5	15
6	Theoretical characterization of the trifluoromethyltrioxy radical. <i>Chemical Physics</i> , 1985, 98, 99-104.	0.9	2
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10	Scaled quantum mechanical (SQM) force field and vibrational assignment for cyclohexane. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1985, 41, 425-433.	0.1	20
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844	Vibrational spectroscopic (FTIR and FT Raman) studies, first order hyperpolarizabilities and HOMO, LUMO analysis of p-toluenesulfonyl isocyanate using ab initio HF and DFT methods. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 81, 711-723.	2.0	37
845	Quantum chemical studies on structure of 1-3-dibromo-5-chlorobenzene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 82, 316-326.	2.0	26
846	Molecular structure, vibrational spectroscopic, first hyperpolarizability, NBO and HOMO, LUMO studies of P-Iodobenzene sulfonyl chloride. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 82, 332-339.	2.0	19
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848	Structural analysis, vibrational spectra and coordinated normal of 2R-(α^{\sim})-6-hydroxytremetone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 84, 111-116.	2.0	24
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946	Vibrational and scaled quantum chemical study of O,O-dimethyl S-methylcarbamoylmethyl phosphorodithioate, dimethoate. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 89, 222-230.	2.0	7
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954	Analysis of vibrational spectra (FT-IR and FT-Raman) and nonlinear optical properties of organic 2-chloro-p-xylene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 94, 36-47.	2.0	13
955	Vanillin and isovanillin: Comparative vibrational spectroscopic studies, conformational stability and NLO properties by density functional theory calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 95, 354-368.	2.0	54
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972	Experimental and computational study on molecular structure and vibrational analysis of 4,5-Bis(hydroxymethyl)-2-methylpyridin-3-ol by normal coordinate treatment. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 115, 191-201.	2.0	9
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