

Sergey V Krasnoshchekov

List of Publications by Year in descending order

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papers

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#	ARTICLE	IF	CITATIONS
1	Numerical-Analytic Implementation of the Higher-Order Canonical Van Vleck Perturbation Theory for the Interpretation of Medium-Sized Molecule Vibrational Spectra. <i>Journal of Physical Chemistry A</i> , 2012, 116, 3691-3709.	2.5	69
2	Structure and vibrational assignment of gauche-1,3-butadiene. <i>Journal of Molecular Structure</i> , 1985, 129, 57-67.	3.6	61
3	Criteria for first- and second-order vibrational resonances and correct evaluation of the Darling-Dennison resonance coefficients using the canonical Van Vleck perturbation theory. <i>Journal of Chemical Physics</i> , 2014, 141, 234114.	3.0	55
4	Determination of the Eckart molecule-fixed frame by use of the apparatus of quaternion algebra. <i>Journal of Chemical Physics</i> , 2014, 140, .	3.0	35
5	An ab initio prediction of structures and vibrational frequencies of high-energy rotamers of glyoxal and acrolein. <i>Chemical Physics</i> , 1988, 125, 63-75.	1.9	32
6	Polyad quantum numbers and multiple resonances in anharmonic vibrational studies of polyatomic molecules. <i>Journal of Chemical Physics</i> , 2013, 139, 184101.	3.0	31
7	Anharmonic Vibrational Analysis of the Gas-Phase Infrared Spectrum of 1,1-Difluoroethylene Using the Operator Van Vleck Canonical Perturbation Theory. <i>Journal of Physical Chemistry A</i> , 2013, 117, 3041-3056.	2.5	30
8	Ab initio structures and vibrational analysis of two planar configurations of 1,3,5-hexatriene. <i>Computational and Theoretical Chemistry</i> , 1986, 148, 131-140.	1.5	29
9	Ab initio structures and vibrational analysis of the isoprene conformers. <i>Journal of Molecular Structure</i> , 1987, 160, 337-346.	3.6	29
10	Ab Initio Anharmonic Analysis of Vibrational Spectra of Uracil Using the Numerical-Analytic Implementation of Operator Van Vleck Perturbation Theory. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6723-6737.	2.5	29
11	Molecular structure and conformation of nitrobenzene reinvestigated by combined analysis of gas-phase electron diffraction, rotational constants, and theoretical calculations. <i>Structural Chemistry</i> , 2007, 18, 739-753.	2.0	28
12	An ab initio structural and vibrational analysis of gauche,trans,trans- and gauche,cis,trans-hexa-1,3,5-trienes. <i>Structural Chemistry</i> , 1992, 3, 15-26.	2.0	27
13	Anharmonic Vibrational Analysis of the Infrared and Raman Gas-Phase Spectra of <i>s-trans</i> - and <i>s-gauche</i> -1,3-Butadiene. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10706-10723.	2.5	27
14	Anharmonic Force Fields and Perturbation Theory in the Interpretation of Vibrational Spectra of Polyatomic Molecules. <i>Russian Journal of Physical Chemistry A</i> , 2008, 82, 592-602.	0.6	21
15	Ab initio analysis of structure and vibrational spectrum of methyl nitrate. <i>Chemical Physics</i> , 1986, 106, 69-73.	1.9	19
16	All ab initio vibrational study of rotational isomerism in oxalyl fluoride, $O=C=CF_2$, and acryloyl fluoride, $O=C=CH_2$. <i>Chemical Physics</i> , 1990, 147, 65-75.	1.9	17
17	Nonempirical Anharmonic Vibrational Perturbation Theory Applied to Biomolecules: Free-Base Porphin. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1616-1627.	2.5	17
18	Transferability of quantum mechanical force field scale factors between conjugated hydrocarbons. <i>Journal of Molecular Structure</i> , 1990, 222, 415-429.	3.6	16

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19	Some aspects of scaling the molecular quantum mechanical force field. <i>Journal of Molecular Structure</i> , 1996, 376, 363-368.	3.6	15
20	Comparing the accuracy of perturbative and variational calculations for predicting fundamental vibrational frequencies of dihalomethanes. <i>Journal of Chemical Physics</i> , 2018, 148, 084102.	3.0	14
21	Rigorous vibrational Fermi resonance criterion revealed: two different approaches yield the same result. <i>Molecular Physics</i> , 2020, 118, e1743887.	1.7	13
22	Force constants and molecular potential functions in redundant coordinates. <i>Journal of Molecular Structure</i> , 1985, 131, 347-356.	3.6	12
23	Ab initio vibrational analysis of three rotamers of 2-propen-1-imine, H ₂ C=CH-CH=N-H, and methanimine, H ₂ C=N-H. <i>Journal of Computational Chemistry</i> , 1988, 9, 443-454.	3.3	12
24	Ab Initio Vibrational Analysis of Cyclopropene, Its Fluoro Derivatives, and Their Deutero Analogues. <i>Journal of Physical Chemistry A</i> , 1998, 102, 2363-2371.	2.5	12
25	Interpretation of vibrational IR spectrum of uracil using anharmonic calculation of frequencies and intensities in second-order perturbation theory. <i>Optics and Spectroscopy (English Translation of) Tj ETQq1 1 0.784614 rgBT /Overlock</i>	1.4	10
26	Determination of accurate semiexperimental equilibrium structure of proline using efficient transformations of anharmonic force fields among the series of isotopologues. <i>Molecular Physics</i> , 2017, 115, 942-951.	1.7	10
27	Theoretical study of some pyrazole derivatives and rare earth metal complexes. <i>Computational and Theoretical Chemistry</i> , 1998, 453, 17-28.	1.5	9
28	Calculation of anharmonic intensities in vibrational spectra of raman scattering and full interpretation of the vibrational spectrum of trans-1,3-butadiene. <i>Moscow University Chemistry Bulletin</i> , 2010, 65, 19-29.	0.6	9
29	Theoretical interpretation of the vibrational spectrum of bicyclo[1.1.0]butane in terms of an ab initio anharmonic model. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2014, 117, 366-373.	0.6	8
30	Potential functions of internal rotation of the methacryloyl fluoride molecule in the ground (S ₀) and excited (S ₁) electronic states. <i>Journal of Molecular Structure</i> , 2019, 1181, 228-234.	3.6	7
31	Internal rotation potential functions of the acryloyl chloride molecule in the ground (S ₀) and excited (S ₁) electronic states. <i>Russian Journal of Physical Chemistry A</i> , 2007, 81, 34-37.	0.6	6
32	Anharmonic vibrational analysis of s-trans and s-cis conformers of acryloyl fluoride using numerical-analytic Van Vleck operator perturbation theory. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 189, 66-79.	3.9	6
33	The determination of the equilibrium geometry of a molecule with the use of microwave data and theoretical rotational-vibrational interaction constants. <i>Russian Journal of Physical Chemistry A</i> , 2006, 80, 1448-1455.	0.6	5
34	Scale factors as effective parameters for correcting nonempirical force fields. <i>Russian Journal of Physical Chemistry A</i> , 2007, 81, 585-592.	0.6	5
35	Ladder operators for Morse oscillator and a perturbed vibrational problem. <i>International Reviews in Physical Chemistry</i> , 2019, 38, 63-113.	2.3	5
36	The internal rotation potential functions of the methacryloyl chloride molecule in the ground and excited electronic states. <i>Russian Journal of Physical Chemistry A</i> , 2009, 83, 962-966.	0.6	4

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37	Analysis of the Structure and Conductivity of Kinked Carbon Chains Obtained by Pulsed Plasma Deposition on Various Metal Substrates. <i>Semiconductors</i> , 2018, 52, 907-913.	0.5	4
38	Fundamental studies of vibrational resonance phenomena by multivalued resummation of the divergent Rayleigh-Schrödinger perturbation theory series: deciphering polyad structures of three $H_2^{16}O$ isotopologues. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 6655-6675.	2.8	4
39	Absolute IR vibrational band intensities of hexafluoroacetone: Comparison of experiment and anharmonic ab initio calculation using the second-order operator canonical Van Vleck perturbation theory. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2018, 217, 243-252.	2.3	3
40	Vibrational spectroscopy of tolane; Coriolis coupling between Raman-active modes of g symmetry. <i>Molecular Physics</i> , 2019, 117, 1059-1068.	1.7	3
41	Disentangling the IR spectra of 2,3,3,3-tetrafluoropropene using an ab initio description of vibrational polyads by means of canonical Van Vleck perturbation theory. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2019, 239, 106656.	2.3	3
42	Normal ordering of the $su(1, 1)$ ladder operators for the quasi-number states of the Morse oscillator. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2020, 384, 126493.	2.1	3
43	Hypofluorous acid (HOF): A molecule with a rare (1,-2,-1) vibrational resonance and (8,3,2) polyad structure revealed by Padé-Hermite resummation of divergent Rayleigh-Schrödinger perturbation theory series. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2021, 268, 107620.	2.3	3
44	Fundamental Analysis of Singular and Resonance Phenomena in Vibrational Polyads of the Difluorosilylene Molecule. <i>Optics and Spectroscopy (English Translation of Optika i Spektroskopiya)</i> , 2020, 128, 1927-1938.	0.6	3
45	Vibrational spectra and conformational composition of ethylene glycol dinitrate in solid phases. <i>Journal of Applied Spectroscopy</i> , 1988, 48, 614-619.	0.7	2
46	Effect of scaling of a quantum mechanical force field on the frequencies and forms of molecular vibrations. <i>Journal of Structural Chemistry</i> , 1998, 39, 169-174.	1.0	2
47	Potential function of the internal rotation of a methacrolein molecule in the ground (S_0) electronic state. <i>Russian Journal of Physical Chemistry A</i> , 2016, 90, 1609-1613.	0.6	2
48	Analysis of the Raman Spectrum of Kinked Carbon Chains Taking into Account the Model of Various End Groups. <i>Journal of Surface Investigation</i> , 2018, 12, 564-569.	0.5	2
49	Overtone spectroscopy of $\nu(C=O)$ stretching vibration of hexafluoroacetone: Experimental and ab initio determination of peak positions, absolute intensities, and band shapes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 238, 118396.	3.9	2
50	Vibrational spectra and calculation of the normal vibrations of 1,3-dimethyl-1,1,3,3-tetrachlorodisiloxane. <i>Journal of Applied Spectroscopy</i> , 1984, 40, 689-692.	0.7	1
51	Structure of the 3,3-dimethyl-3-silathietane molecule according to data from gas-phase electron diffraction analysis with consideration of vibrational effects. <i>Journal of Structural Chemistry</i> , 1988, 28, 674-679.	1.0	0
52	Infrared vibrational spectra and absolute intensities of fundamental bands of bis(trifluoromethyl)ketene: ab initio interpretation using the second order operator Van Vleck perturbation theory. <i>Journal of Quantitative Spectroscopy and Radiative Transfer</i> , 2021, 276, 107952.	2.3	0