Sergey V Krasnoshchekov

List of Publications by Year
in descending order

52	771	516215 16	552369 26
papers	citations	h-index	g-index

52	52	52	424
all docs	docs citations	times ranked	citing authors

#	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. Journal of Physical Chemistry A, 2012, 116, 3691-3709.	1.1	69
2	Structure and vibrational assignment of gouche-1,3-butadiene. Journal of Molecular Structure, 1985, 129, 57-67.	1.8	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. Journal of Chemical Physics, 2014, 141, 234114.	1.2	55
4	Determination of the Eckart molecule-fixed frame by use of the apparatus of quaternion algebra. Journal of Chemical Physics, 2014, 140, .	1.2	35
5	An ab initio prediction of structures and vibrational frequencies of high-energy rotamers of glyoxal and acrolein. Chemical Physics, 1988, 125, 63-75.	0.9	32
6	Polyad quantum numbers and multiple resonances in anharmonic vibrational studies of polyatomic molecules. Journal of Chemical Physics, 2013, 139, 184101.	1.2	31
7	Anharmonic Vibrational Analysis of the Gas-Phase Infrared Spectrum of 1,1-Difluoroethylene Using the Operator Van Vleck Canonical Perturbation Theory. Journal of Physical Chemistry A, 2013, 117, 3041-3056.	1.1	30
8	Ab initio structures and vibrational analysis of two planar configurations of 1,3,5-hexatriene. Computational and Theoretical Chemistry, 1986, 148, 131-140.	1.5	29
9	Ab initio structures and vibrational analysis of the isoprene conformers. Journal of Molecular Structure, 1987, 160, 337-346.	1.8	29
10	Ab Initio Anharmonic Analysis of Vibrational Spectra of Uracil Using the Numerical-Analytic Implementation of Operator Van Vleck Perturbation Theory. Journal of Physical Chemistry A, 2015, 119, 6723-6737.	1.1	29
11	Molecular structure and conformation of nitrobenzene reinvestigated by combined analysis of gas-phase electron diffraction, rotational constants, and theoretical calculations. Structural Chemistry, 2007, 18, 739-753.	1.0	28
12	An ab initio structural and vibrational analysis of gauche,trans,trans- and gauche,cis,trans-hexa-1,3,5-trienes. Structural Chemistry, 1992, 3, 15-26.	1.0	27
13	Anharmonic Vibrational Analysis of the Infrared and Raman Gas-Phase Spectra of s-trans- and s-gauche-1,3-Butadiene. Journal of Physical Chemistry A, 2015, 119, 10706-10723.	1.1	27
14	Anharmonic Force Fields and Perturbation Theory in the Interpretation of Vibrational Spectra of Polyatomic Molecules. Russian Journal of Physical Chemistry A, 2008, 82, 592-602.	0.1	21
15	Ab initio analysis of structure and vibrational spectrum of methyl nitrate. Chemical Physics, 1986, 106, 69-73.	0.9	19
16	All ab initio vibrational study of rotational isomerism in oxalyl fluoride, Oî—»CF-CFî—»O, and acryloyl fluoride, Oî—»CF-CHî—»CH2. Chemical Physics, 1990, 147, 65-75.	0.9	17
17	Nonempirical Anharmonic Vibrational Perturbation Theory Applied to Biomolecules: Free-Base Porphin. Journal of Physical Chemistry A, 2015, 119, 1616-1627.	1.1	17
18	Transferability of quantum mechanical force field scale factors between conjugated hydrocarbons. Journal of Molecular Structure, 1990, 222, 415-429.	1.8	16

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19	Some aspects of scaling the molecular quantum mechanical force field. Journal of Molecular Structure, 1996, 376, 363-368.	1.8	15
20	Comparing the accuracy of perturbative and variational calculations for predicting fundamental vibrational frequencies of dihalomethanes. Journal of Chemical Physics, 2018, 148, 084102.	1.2	14
21	Rigorous vibrational Fermi resonance criterion revealed: two different approaches yield the same result. Molecular Physics, 2020, 118, e1743887.	0.8	13
22	Force constants and molecular potential functions in redundant coordinates. Journal of Molecular Structure, 1985, 131, 347-356.	1.8	12
23	Ab initio vibrational analysis of three rotamers of 2-propen-1-imine, H2C?CH?HC?N?H, and methanimine, H2C?N?H. Journal of Computational Chemistry, 1988, 9, 443-454.	1.5	12
24	Ab Initio Vibrational Analysis of Cyclopropene, Its Fluoro Derivatives, and Their Deutero Analogues. Journal of Physical Chemistry A, 1998, 102, 2363-2371.	1.1	12
25	Interpretation of vibrational IR spectrum of uracil using anharmonic calculation of frequencies and intensities in second-order perturbation theory. Optics and Spectroscopy (English Translation of) Tj ETQq1 1 0.784314 rgBT /Overlock	0.2	10
26	Determination of accurate semiexperimental equilibrium structure of proline using efficient transformations of anharmonic force fields among the series of isotopologues. Molecular Physics, 2017, 115, 942-951.	0.8	10
27	Theoretical study of some pyrazole derivatives and rare earth metal complexes. Computational and Theoretical Chemistry, 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. Moscow University Chemistry Bulletin, 2010, 65, 19-29.	0.2	9
29	Theoretical interpretation of the vibrational spectrum of bicyclo[1.1.0]butane in terms of an ab initio anharmonic model. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2014, 117, 366-373.	0.2	8
30	Potential functions of internal rotation of the methacryloyl fluoride molecule in the ground (S0) and excited (S1) electronic states. Journal of Molecular Structure, 2019, 1181, 228-234.	1.8	7
31	Internal rotation potential functions of the acryloyl chloride molecule in the ground (S 0) and excited (S 1) electronic states. Russian Journal of Physical Chemistry A, 2007, 81, 34-37.	0.1	6
32	Anharmonic vibrational analysis of s-trans and s-cis conformers of acryloyl fluoride using numerical-analytic Van Vleck operator perturbation theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 189, 66-79.	2.0	6
33	The determination of the equilibrium geometry of a molecule with the use of microwave data and theoretical rotational-vibrational interaction constants. Russian Journal of Physical Chemistry A, 2006, 80, 1448-1455.	0.1	5
34	Scale factors as effective parameters for correcting nonempirical force fields. Russian Journal of Physical Chemistry A, 2007, 81, 585-592.	0.1	5
35	Ladder operators for Morse oscillator and a perturbed vibrational problem. International Reviews in Physical Chemistry, 2019, 38, 63-113.	0.9	5
36	The internal rotation potential functions of the methacryloyl chloride molecule in the ground and excited electronic states. Russian Journal of Physical Chemistry A, 2009, 83, 962-966.	0.1	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. Semiconductors, 2018, 52, 907-913.	0.2	4
38	Fundamental studies of vibrational resonance phenomena by multivalued resummation of the divergent Rayleighâ€“SchrÃ¶dinger perturbation theory series: deciphering polyad structures of three H₂¹⁶O isotopologues. Physical Chemistry Chemical Physics, 2022, 24, 6655-6675.	1.3	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. Journal of Quantitative Spectroscopy and Radiative Transfer, 2018, 217, 243-252.	1.1	3
40	Vibrational spectroscopy of tolane; Coriolis coupling between Raman-active modes of g symmetry. Molecular Physics, 2019, 117, 1059-1068.	0.8	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. Journal of Quantitative Spectroscopy and Radiative Transfer, 2019, 239, 106656.	1.1	3
42	Normal ordering of the su(1, 1) ladder operators for the quasi-number states of the Morse oscillator. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126493.	0.9	3
43	Hypofluorous acid (HOF): A molecule with a rare (1,-2,-1) vibrational resonance and (8,3,2) polyad structure revealed by PadÃ©-Hermite resummation of divergent Rayleigh-SchrÃ¶dinger perturbation theory series. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 268, 107620.	1.1	3
44	Fundamental Analysis of Singular and Resonance Phenomena in Vibrational Polyads of the Difluorosilylene Molecule. Optics and Spectroscopy (English Translation of Optika I Spektroskopiya), 2020, 128, 1927-1938.	0.2	3
45	Vibrational spectra and conformational composition of ethylene glycol dinitrate in solid phases. Journal of Applied Spectroscopy, 1988, 48, 614-619.	0.3	2
46	Effect of scaling of a quantum mechanical force field on the frequencies and forms of molecular vibrations. Journal of Structural Chemistry, 1998, 39, 169-174.	0.3	2
47	Potential function of the internal rotation of a methacrolein molecule in the ground (S 0) electronic state. Russian Journal of Physical Chemistry A, 2016, 90, 1609-1613.	0.1	2
48	Analysis of the Raman Spectrum of Kinked Carbon Chains Taking into Account the Model of Various End Groups. Journal of Surface Investigation, 2018, 12, 564-569.	0.1	2
49	Overtone spectroscopy of ν(C=O) stretching vibration of hexafluoroacetone: Experimental and ab initio determination of peak positions, absolute intensities, and band shapes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 238, 118396.	2.0	2
50	Vibrational spectra and calculation of the noemal vibrations of 1,3-dimethyl-1,1,3,3-tetrachlorodisiloxane. Journal of Applied Spectroscopy, 1984, 40, 689-692.	0.3	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. Journal of Structural Chemistry, 1988, 28, 674-679.	0.3	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. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 276, 107952.	1.1	0