Sergey V Krasnoshchekov

List of Publications by Year
in descending order

52	771	516710 16	552781 26
papers	citations	h-index	g-index

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

#	Article	IF	Citations
1	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.	2.8	4
2	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.	2.3	3
3	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.	2.3	0
4	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.	2.1	3
5	Rigorous vibrational Fermi resonance criterion revealed: two different approaches yield the same result. Molecular Physics, 2020, 118, e1743887.	1.7	13
6	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.	3.9	2
7	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.	0.6	3
8	Vibrational spectroscopy of tolane; Coriolis coupling between Raman-active modes of g symmetry. Molecular Physics, 2019, 117, 1059-1068.	1.7	3
9	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.	2.3	3
10	Ladder operators for Morse oscillator and a perturbed vibrational problem. International Reviews in Physical Chemistry, 2019, 38, 63-113.	2.3	5
11	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.	3.6	7
12	Comparing the accuracy of perturbative and variational calculations for predicting fundamental vibrational frequencies of dihalomethanes. Journal of Chemical Physics, 2018, 148, 084102.	3.0	14
13	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.	3.9	6
14	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.	0.5	2
15	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.	2.3	3
16	Analysis of the Structure and Conductivity of Kinked Carbon Chains Obtained by Pulsed Plasma Deposition on Various Metal Substrates. Semiconductors, 2018, 52, 907-913.	0.5	4
17	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.	1.7	10
18	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.	0.6	2

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19	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.	2.5	29
20	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.	2.5	27
21	Nonempirical Anharmonic Vibrational Perturbation Theory Applied to Biomolecules: Free-Base Porphin. Journal of Physical Chemistry A, 2015, 119, 1616-1627.	2.5	17
22	Determination of the Eckart molecule-fixed frame by use of the apparatus of quaternion algebra. Journal of Chemical Physics, 2014, 140, .	3.0	35
23	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.	3.0	55
24	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.	0.6	8
25	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.	2.5	30
26	Polyad quantum numbers and multiple resonances in anharmonic vibrational studies of polyatomic molecules. Journal of Chemical Physics, 2013, 139, 184101.	3.0	31
27	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.	2.5	69
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.	0.6	9
29	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		
30	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.	0.6	4
31	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.	0.6	21
32	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.	0.6	6
33	Scale factors as effective parameters for correcting nonempirical force fields. Russian Journal of Physical Chemistry A, 2007, 81, 585-592.	0.6	5
34	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.	2.0	28
35	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.	0.6	5
36	Theoretical study of some pyrazole derivatives and rare earth metal complexes. Computational and Theoretical Chemistry, 1998, 453, 17-28.	1.5	9

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37	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.	1.0	2
38	Ab Initio Vibrational Analysis of Cyclopropene, Its Fluoro Derivatives, and Their Deutero Analogues. Journal of Physical Chemistry A, 1998, 102, 2363-2371.	2.5	12
39	Some aspects of scaling the molecular quantum mechanical force field. Journal of Molecular Structure, 1996, 376, 363-368.	3.6	15
40	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.	2.0	27
41	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.	1.9	17
42	Transferability of quantum mechanical force field scale factors between conjugated hydrocarbons. Journal of Molecular Structure, 1990, 222, 415-429.	3.6	16
43	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.	3.3	12
44	Vibrational spectra and conformational composition of ethylene glycol dinitrate in solid phases. Journal of Applied Spectroscopy, 1988, 48, 614-619.	0.7	2
45	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.	1.0	0
46	An ab initio prediction of structures and vibrational frequencies of high-energy rotamers of glyoxal and acrolein. Chemical Physics, 1988, 125, 63-75.	1.9	32
47	Ab initio structures and vibrational analysis of the isoprene conformers. Journal of Molecular Structure, 1987, 160, 337-346.	3.6	29
48	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
49	Ab initio analysis of structure and vibrational spectrum of methyl nitrate. Chemical Physics, 1986, 106, 69-73.	1.9	19
50	Structure and vibrational assignment of gouche-1,3-butadiene. Journal of Molecular Structure, 1985, 129, 57-67.	3.6	61
51	Force constants and molecular potential functions in redundant coordinates. Journal of Molecular Structure, 1985, 131, 347-356.	3.6	12
52	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.	0.7	1