

Igor S Ignatyev

List of Publications by Year in descending order

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94
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docs citations

94
times ranked

847
citing authors

#	ARTICLE	IF	CITATIONS
1	Mechanism of the C ₂ H ₅ +O ₂ reaction. Journal of Chemical Physics, 1997, 107, 141-155.	1.2	142
2	Binuclear Homoleptic Nickel Carbonyls: Incorporation of Ni ²⁺ Ni Single, Double, and Triple Bonds, Ni ₂ (CO) _x (x= 5, 6, 7). Journal of the American Chemical Society, 2000, 122, 1989-1994.	6.6	61
3	Theoretical prediction of vibrational spectra. The a priori scaled quantum mechanical (SQM) force field and vibrational spectra of pyrimidine. Spectrochimica Acta Part A: Molecular Spectroscopy, 1992, 48, 111-119.	0.1	52
4	Competitive ring hydride shifts and tolyl-benzyl rearrangements in tolyl and silatolyl cations. Chemical Physics Letters, 2000, 326, 101-108.	1.2	45
5	[7]Circulene: a remarkably floppy polycyclic aromatic C ₂₈ H ₁₄ isomer. The Journal of Physical Chemistry, 1993, 97, 3212-3216.	2.9	39
6	Vibrational spectra and molecular structure of methyl vinyl ether. Journal of Molecular Structure, 1981, 72, 25-39.	1.8	34
7	Triethanolammonium salicylate " Protic alkanolammonium ionic liquid. Journal of Molecular Liquids, 2016, 221, 1218-1224.	2.3	33
8	Stable Hexacoordinated Neutral Complexes between Silyl Halides and Two Water or Two Ammonia Molecules: SiX ₄ Y ₂ (X = H, F, Cl; Y = H ₂ O, NH ₃). Journal of Physical Chemistry A, 2001, 105, 7665-7671.	1.1	27
9	Vibrational spectra of trimethylsilanol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 1169-1178.	2.0	26
10	Molecular structure, force field and vibrational spectra of tetramethoxysilane. Journal of Molecular Structure, 1991, 244, 193-202.	1.8	24
11	Effect of the Silyl Substitution on Structure and Vibrational Spectra of Hydrogen-Bonded Networks in Dimers, Cyclic Trimers, and Tetramers. Journal of Physical Chemistry A, 2002, 106, 11644-11652.	1.1	21
12	Bonding in germatranyl cation and germatranes. Journal of Organometallic Chemistry, 2007, 692, 5697-5700.	0.8	21
13	Vibrational spectra and structure of methoxysilanes and products of their hydrolysis. Vibrational Spectroscopy, 2006, 40, 1-9.	1.2	19
14	Structure and Vibrational Spectra of Ti(IV) Hydroxides and Their Clusters with Expanded Titanium Coordination. DFT Study. Journal of Physical Chemistry A, 2007, 111, 7973-7979.	1.1	19
15	The vibrational spectrum and chemical constitution of trimethylsilylvinyl ether, (CH ₃) ₃ SiOCH=CH ₂ . Spectrochimica Acta Part A: Molecular Spectroscopy, 1971, 27, 2291-2308.	0.1	18
16	Diazasilene (Si ₂ N ₂): a comparison of coupled cluster methods with experiment and local density functional methods. The Journal of Physical Chemistry, 1992, 96, 7632-7634.	2.9	18
17	Role of Hexacoordinated Silicon Intermediates in the Hydrolysis and Racemization Reactions of Silyl Halides. Organometallics, 2001, 20, 3113-3121.	1.1	17
18	Theoretical study of the mechanisms of the hydrolysis and condensation reactions of silicon and titanium alkoxides: similarities and differences. Dalton Transactions, 2010, 39, 6967.	1.6	17

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19	Potential Energy Surface of the Dimethylsilylium Cation and Mechanism of the Isomer Interconversion. <i>Organometallics</i> , 1996, 15, 5674-5677.	1.1	16
20	Intramolecular hydrogen bonding in silanediols. <i>Computational and Theoretical Chemistry</i> , 2004, 678, 249-256.	1.5	16
21	Hydrogen bonding and structure of silanediol dimers and tetramers. <i>Chemical Physics Letters</i> , 2004, 384, 326-331.	1.2	16
22	Vibrational spectra of silatranes and germatranes $\text{XM}(\text{OCH}_2\text{CH}_2)_3\text{N}$ ($\text{X}=\text{F},\text{Cl},\text{H}$; $\text{M}=\text{Si},\text{Ge}$). The problem of the theoretical prediction of condensed phase spectra. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 95, 37-45.	2.0	16
23	The ab initio analysis of molecular geometry and force fields in H_3XOXH_3 ($\text{X} = \text{C}, \text{Si}$) series. <i>Journal of Molecular Structure</i> , 1988, 172, 139-149.	1.8	15
24	Effects of Fluorination on Methylene Insertion Reactions. <i>Journal of the American Chemical Society</i> , 1997, 119, 12306-12310.	6.6	15
25	Dihydrogen and Methane Elimination from Adducts Formed by the Interaction of Carbenium and Silylium Cations with Nucleophiles. <i>Journal of the American Chemical Society</i> , 2004, 126, 14515-14526.	6.6	15
26	Bromine Halides: The Neutral Molecules BrClF_n ($n = 1\text{--}5$) and Their Anions Structures, Energetics, and Electron Affinities. <i>Journal of the American Chemical Society</i> , 1999, 121, 6904-6910.	6.6	13
27	Condensation reactions in silanol water clusters. <i>Chemical Physics Letters</i> , 2003, 368, 616-624.	1.2	13
28	Vibrational spectrum of methoxytrimethylsilane. <i>Journal of Molecular Structure</i> , 2005, 744-747, 331-338.	1.8	13
29	Vibrational spectrum of chlorotrimethylsilane. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 62, 293-301.	2.0	12
30	Quantum-chemical study of the stereoelectronic structure of 1-fluorosilatrane, 1,1-difluoroquasisilatrane, 1,1,1-trifluorohyposilatrane, and cations formed thereof. <i>Russian Journal of General Chemistry</i> , 2010, 80, 2274-2282.	0.3	12
31	Nucleogenic silylium cations and their analogs. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 1331-1340.	0.8	12
32	Structure and vibrational spectra of vinyl ether conformers. The comparison of B3LYP and MP2 predictions. <i>Chemical Physics</i> , 2007, 333, 148-156.	0.9	11
33	Radiochemical study of the gas phase reaction of nucleogenic diethylsilylium ions with methanol and butanol. <i>Journal of Organometallic Chemistry</i> , 2002, 656, 258-261.	0.8	10
34	Mechanism of Rearrangement and Alkene Addition/Elimination Reactions of SiC_3H_9^+ . <i>Organometallics</i> , 1998, 17, 2819-2824.	1.1	9
35	Rearrangement and decomposition of $(\text{CH}_3)_3\text{M}^+$ ($\text{M}=\text{Si}, \text{Ge}, \text{Sn}$) ions: A DFT study. <i>Journal of Organometallic Chemistry</i> , 2008, 693, 2856-2862.	0.8	9
36	Effect of substituents and hydrogen bonding on barrier heights in dehydration reactions of carbon and silicon geminal diols. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 18507.	1.3	9

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37	Scaled ab initio force fields of s-cis and skew conformers of methyl vinyl ether. <i>Journal of Molecular Structure</i> , 1991, 246, 279-287.	1.8	8
38	Ab initio study of trimethyloxonium and disilylmethyloxonium cations as intermediates in reactions of CH ₃ cations with ethers and disiloxanes. <i>Computational and Theoretical Chemistry</i> , 1991, 236, 249-257.	1.5	8
39	Intramolecular coordination of silicon in silyl formates: spectroscopic evidence confirmed by ab initio calculations. <i>Journal of Molecular Structure</i> , 1991, 245, 139-145.	1.8	8
40	Transition states for inversion and retention of configuration channels in the reactions of alkyl and silyl fluorides with a water molecule. <i>Chemical Physics Letters</i> , 2000, 320, 469-474.	1.2	8
41	Structures and mutual transformations of isomers of germylium ions (CH ₃) ₂ Ge ⁺ and (CH ₃) ₂ HGe ⁺ and their silicon analogs. <i>Russian Journal of General Chemistry</i> , 2007, 77, 575-580.	0.3	8
42	Mechanism of the Catalytic Activity of Nucleophiles in the Stepwise Hydrolysis and Condensation Reactions of Tetramethoxysilane. <i>ChemPhysChem</i> , 2009, 10, 940-945.	1.0	7
43	DFT predictions of vibrational spectra of titanium tetramethoxide oligomers and the structure of titanium tetraalkoxides in liquid and solid phases. <i>Vibrational Spectroscopy</i> , 2009, 51, 218-225.	1.2	7
44	Role of structures with penta- and hexacoordinate silicon in the nucleophile-catalyzed hydrolysis of tetramethoxysilane. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 841-847.	1.3	7
45	An assessment of DFT methods for predicting the thermochemistry of ion-molecule reactions of group 14 elements (Si, Ge, Sn). <i>Journal of Molecular Modeling</i> , 2013, 19, 5439-5444.	0.8	7
46	Vibrational spectra and electronic structure of germatranols (HO) ₄ Ge(OCH ₂ CH ₂) _n NR ₃ (R=H); <i>J. Phys. Chem. B</i> , 2008, 112, 10000-10008.	0.8	7
47	DFT study of the hydrolysis reaction in atranones and ocanones: the influence of transannular bonding. <i>Journal of Molecular Modeling</i> , 2016, 22, 3.	0.8	7
48	Vibrational spectrum and molecular structure of methoxyallene. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1990, 46, 1505-1512.	0.1	6
49	Reactions of Phenyl Cations with Methanol and Methyl Fluoride. <i>Journal of Physical Chemistry A</i> , 2001, 105, 4535-4540.	1.1	6
50	Theoretical models for the description of the IR frequency shifts of carbon monoxide interacting with silanol groups. <i>Chemical Physics Letters</i> , 2005, 406, 273-278.	1.2	6
51	Structure and vibrational spectra of dimethylsilanediol and methylsilanetriol dimers. <i>Chemical Physics Letters</i> , 2005, 412, 359-364.	1.2	6
52	Quantum chemical study of silanediols as metal binding groups for metalloprotease inhibitors. <i>Journal of Molecular Modeling</i> , 2013, 19, 1819-1834.	0.8	6
53	Molecular and crystal structures of 2-phenyl-2-hydro-6-methyl-1,3-dioxo-6-aza-2-silacyclooctane. <i>Journal of Molecular Structure</i> , 2015, 1094, 169-173.	1.8	6
54	The relation of methoxy group CH bond lengths and stretching frequencies to the oxygen lone pair orientation. <i>Journal of Molecular Structure</i> , 1989, 197, 251-257.	1.8	5

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55	Vibrational spectra of hexafluorodisiloxane and internal rotation around the SiO bond. An ab initio study. <i>Computational and Theoretical Chemistry</i> , 1995, 343, 69-75.	1.5	4
56	The search for the low-lying states of the silicon carbide cluster cation Si ₂ C ⁺ . <i>Journal of Chemical Physics</i> , 1995, 103, 7025-7029.	1.2	4
57	Synthesis and characterization of hypercoordinated germanium complexes with hydroxyalkylethylenediamines. <i>Journal of Organometallic Chemistry</i> , 2021, 958, 122188.	0.8	4
58	Vibrational spectrum, force field, and chemical structure of bis(trimethylsilyl) peroxide. <i>Journal of Structural Chemistry</i> , 1985, 26, 201-207.	0.3	3
59	Normal coordinate analysis of the vibrational spectra of stannatranes. <i>Spectrochimica Acta Part A: Molecular Spectroscopy</i> , 1992, 48, 489-493.	0.1	3
60	Silacyanogen. <i>Journal of Chemical Physics</i> , 1997, 107, 5776-5779.	1.2	3
61	Comment on: "Reactions of Phenyl Cations with Methanol and Methyl Fluoride". <i>Journal of Physical Chemistry A</i> , 2002, 106, 7076-7077.	1.1	3
62	Ion-Molecular Reactions of Diethylsilylium Ions with Alcohols in the Gas Phase. <i>Russian Journal of General Chemistry</i> , 2003, 73, 61-65.	0.3	3
63	Interconversion of Silylphenyl and Phenylsilyl Cations in the Reaction with Benzene. <i>Russian Journal of General Chemistry</i> , 2005, 75, 1393-1394.	0.3	3
64	Rearrangements of [C ₆ H ₇ Si] ⁺ Cations. A Radiochemical and Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6028-6033.	1.1	3
65	Synthesis of phenylsilane tritium-labeled at the benzene ring. <i>Russian Journal of General Chemistry</i> , 2014, 84, 2125-2129.	0.3	3
66	Vibrational spectrum and intramolecular coordination of silicon in 1-hydrosilatrane. <i>Bulletin of the Academy of Sciences of the USSR Division of Chemical Science</i> , 1986, 35, 1375-1382.	0.0	2
67	Vibrational spectra and structure of X ₃ AlOPX ₃ (X = F, Cl). <i>Journal of Molecular Structure</i> , 1999, 480-481, 667-676.	1.8	2
68	Gas-Phase Ion-Molecular Reactions of Free Ethylsilylium Ions with Ethylene. <i>Russian Journal of General Chemistry</i> , 2001, 71, 206-209.	0.3	2
69	Gas-phase reaction of phenyl cation with diethylamine. <i>Journal of Radioanalytical and Nuclear Chemistry</i> , 2002, 253, 435-437.	0.7	2
70	A Radiochemical Study of Reactions of Diethylsilylium Ions with Trimethyl(tert-butylamino)silane in Gas and Liquid Phases. <i>Russian Journal of General Chemistry</i> , 2005, 75, 69-72.	0.3	2
71	Gas-Phase Reaction of Free Diethylsilylium Ions with Hexamethyldisiloxane. <i>Russian Journal of General Chemistry</i> , 2005, 75, 708-710.	0.3	2
72	Proton Migration in Benzene Complexes of Methyl and Silyl Cations. <i>Russian Journal of General Chemistry</i> , 2005, 75, 1221-1224.	0.3	2

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73	Effect of the Electronic Structure of Carbenium and Silylium Ions on Their Chemical Behavior. Russian Journal of General Chemistry, 2005, 75, 1225-1229.	0.3	2
74	Radiochemical and Quantum-Chemical Study of the Migration of the Cationic Center in the SiC ₆ H ₇ ⁺ Ion. Russian Journal of General Chemistry, 2005, 75, 1395-1398.	0.3	2
75	Reactions of silylium ions with nucleophiles. Russian Journal of General Chemistry, 2006, 76, 1774-1777.	0.3	2
76	Isomerization of silicenium and germanium ions in the systems C ₄ H ₁₁ M ⁺ (M = Si, Ge). Russian Journal of General Chemistry, 2010, 80, 1283-1287.	0.3	2
77	Vibrational spectra and electronic structure of 1-germatranol, 1,1-quasi-germatrandiole, and 1,1,1-hypogermatrantriole (HO) ₄ ⁿ Ge(OCH ₂ CH ₂) _n NR ₃ ⁿ (R = H, Me; n = 1-3). Journal of Structural Chemistry, 2014, 55, 431-437.	0.3	2
78	Force constants and bond lengths in oxygen compounds of silicon, germanium, and phosphorus. Journal of Structural Chemistry, 1976, 16, 541-544.	0.3	1
79	Normal coordinates of the hexafluorodisiloxane molecule F ₃ SiOSiF ₃ and the structure of the vibrational bands of its siloxane bridge. Journal of Applied Spectroscopy, 1978, 28, 321-326.	0.3	1
80	Equilibrium geometry, force field, and electronic structure of the ketene molecule. Journal of Structural Chemistry, 1985, 26, 345-350.	0.3	1
81	Triplet states of carbenium and silylium cations. Chemical Physics Letters, 2001, 337, 158-168.	1.2	1
82	Title is missing!. Russian Journal of General Chemistry, 2001, 71, 934-938.	0.3	1
83	Reply to Comment on "Reactions of Phenyl Cations with Methanol and Methyl Fluoride". Journal of Physical Chemistry A, 2002, 106, 7078-7079.	1.1	1
84	Energies of Association of Carbenium and Silylium Cations with Oxygen-Containing Molecules. Russian Journal of General Chemistry, 2005, 75, 711-713.	0.3	1
85	Radiochemical Study of the Reactions of Diethylsilylium Ions with Hexamethyldisilazane and Isobutylamine in the Gas Phase. Russian Journal of General Chemistry, 2005, 75, 1399-1401.	0.3	1
86	Radiochemical study of gas-phase reactions of diethylstannilium cations Et ₂ SnT ⁺ with oxygen-containing compounds: I. Interaction of diethylstannilium cations with methyl tert-butyl ether. Russian Journal of General Chemistry, 2013, 83, 938-942.	0.3	1
87	Normal vibrations and force field of hexachlorodisiloxane Cl ₃ SiOSiCl ₃ . Journal of Applied Spectroscopy, 1978, 28, 214-218.	0.3	0
88	Vibrational spectrum, force field, and characteristics of the chemical structure of trimethylsilyl formate. Journal of Applied Spectroscopy, 1979, 30, 209-214.	0.3	0
89	Varying metric method in the gradient solution of the inverse mechanical problem of molecular vibrations. Journal of Applied Spectroscopy, 1984, 40, 711-716.	0.3	0
90	Synthesis, molecular structure, and vibrational spectra of tetrakis(2-hydroxyethylammonium) chloride and its triethanolamine precursor and metabolite. Russian Journal of General Chemistry, 2014, 84, 1904-1908.	0.3	0

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91	Radiochemical study of gas-phase reactions of diethylstannyl cations Et_2SnT^+ with oxygen-containing compounds: II. Reaction of diethylstannyl cations with butanol. Russian Journal of General Chemistry, 2014, 84, 816-821.	0.3	0