Valeri I Kovalenko

List of Publications by Year
in descending order

108	1,161	430874	477307
papers	citations	18 h-index	29 g-index

108	108	108	1149
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Investigation of H-bonding of p-(3-carboxymethyl-1-adamantyl)calix[6]arene by IR spectroscopy. Journal of Molecular Structure, 2022, 1248, 131472.	3.6	1
2	Radical character of non-IPR isomer 17418 (C1) of fullerene C76. Fullerenes Nanotubes and Carbon Nanostructures, 2021, 29, 678-684.	2.1	1
3	Substructural Approach for Assessing the Stability of Higher Fullerenes. International Journal of Molecular Sciences, 2021, 22, 3760.	4.1	10
4	Fullerenes C100 and C108: new substructures of higher fullerenes. Structural Chemistry, 2021, 32, 2283-2290.	2.0	0
5	In silico exploration of O-Hâ€¦X2+ (XÂ=ÂCu, Ag, Hg) interaction, targeted adsorption zone, charge density iso-surface, O-H proton analysis and topographic parameters theory for calix[6]arene and calix[8]arene as model. Journal of Molecular Liquids, 2021, 334, 116127.	4.9	13
6	Study of p-(3-carboxymethyl-1-adamantyl)calix[4]arene and tetrapropoxy-p-(3-carboxymethyl-1-adamantyl)calix[4]arene by vibrational spectroscopy and DFT. Journal of Molecular Structure, 2021, 1239, 130508.	3.6	0
7	Comparative study of the vibrational spectra of carboxylate azocalix[4]arenes and azothiacalix[4]arenes. Journal of Molecular Structure, 2021, 1241, 130662.	3.6	1
8	DFT study of conformation, hydrogen bonds, IR, and Raman spectra of the sodium salt of p-hexasulfonatocalix[6]arene DFT. Journal of Molecular Structure, 2021, 1243, 130892.	3.6	5
9	Open-shell nature of non-IPR fullerene Ð¡40: isomers 29 (C2) and 40 (Td). Journal of Molecular Modeling, 2021, 27, 22.	1.8	5
10	Vibrational spectra study of p-sulfonatocalix[4]arene containing azobenzene groups. Journal of Molecular Structure, 2020, 1200, 127058.	3.6	9
11	FT-IR and FT-Raman study of p-sulfonatocalix [8]arene. Journal of Molecular Structure, 2020, 1203, 127474.	3.6	8
12	Features of molecular structure of small non-IPR fullerenes: the two isomers of C50. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	6
13	The key feature of instability of small non-IPR closed-shell fullerenes: three isomers of C40. Mendeleev Communications, 2020, 30, 725-727.	1.6	4
14	Zn and Co redox active coordination polymers as efficient electrocatalysts. Dalton Transactions, 2019, 48, 3601-3609.	3.3	41
15	Investigation of hydrogen bonding in p-sulfonatocalix[4]arene and its thermal stability by vibrational spectroscopy. Journal of Molecular Structure, 2019, 1195, 403-410.	3.6	9
16	Ythrene: From the Real Radical Fullerene Substructure to Hypothetical (yet?) Radical Molecules. Journal of Physical Chemistry C, 2019, 123, 1954-1959.	3.1	6
17	Synthesis and study of the vibrational spectra of a first generation phosphorus-containing dendrimer with pyridyl functional groups. Journal of Molecular Structure, 2018, 1162, 1-9.	3.6	3
18	IR and UV study of reversible water-induced structural transformations of poly(manganese) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 67 Td of Molecular Structure, 2018, 1166, 237-242.	3.6	14

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19	FT-IR and FT-Raman study of hydrogen bonding in p-alkylcalix[8]arenes. Vibrational Spectroscopy, 2018, 95, 38-43.	2.2	20
20	Radical IPR Fullerenes C₇₄ (D_{3h}) and C₇₆ (T_d): Dimer, Trimer, etc. Experiments and Theory. Journal of Physical Chemistry C, 2018, 122, 3146-3151.	3.1	8
21	Vibrational spectroscopic study of cationic phosphorus dendrimers with aminoethylpiperidine terminal groups. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 194, 211-221.	3.9	2
22	Investigation of the structure and hydrogen bonds in adamantylcalix[6]arene by IR spectroscopy and DFT. Vibrational Spectroscopy, 2018, 96, 60-66.	2.2	0
23	Investigation of the conformation and hydrogen bonds in adamantylthiacalix[4]arene by IR spectroscopy and DFT. Journal of Molecular Structure, 2018, 1171, 207-213.	3.6	5
24	Vibrational spectroscopic investigation of the gold complexation within the cascade structure of phosphorus-containing dendrimer. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 203, 118-126.	3.9	3
25	Stabilization of IPR open-shell fullerenes C₇₄ (D_{3h}) and C₇₆ (T_d) in radical addition reactions. Fullerenes Nanotubes and Carbon Nanostructures, 2017, 25, 128-132.	2.1	5
26	Molecular structures of the open-shell IPR isomers of fullerene C90. Fullerenes Nanotubes and Carbon Nanostructures, 2017, 25, 179-184.	2.1	4
27	DFT study of structure, IR and Raman spectra of the first generation dendrimer built from cyclotriphosphazene core with terminal pyrazine groups. Vibrational Spectroscopy, 2017, 92, 54-61.	2.2	4
28	Cyclic cooperative intramolecular hydrogen bond in p-tert-butylcalix[6]arene according to FTIR spectroscopy and DFT studies. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 181, 98-108.	3.9	9
29	DFT study of IR and Raman spectra of phosphotrihydrazone dendrimer with terminal phenolic groups. Journal of Molecular Structure, 2017, 1144, 466-472.	3.6	2
30	Vibrational spectroscopic study on polycationic phosphorus dendrimers. Vibrational Spectroscopy, 2017, 93, 65-77.	2.2	1
31	Vibrational spectra and DFT studies of conjugation in poly(phosphorhydrazone) dendrimers. Vibrational Spectroscopy, 2017, 88, 14-26.	2.2	2
32	DFT study of hydrogen bonding and IR spectra of calix[6]arene. Journal of Molecular Structure, 2017, 1128, 439-447.	3.6	24
33	Structure, IR and Raman spectra of phosphotrihydrazide studied by DFT. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 166, 19-24.	3.9	8
34	Reversible Water-Induced Structural and Magnetic Transformations and Selective Water Adsorption Properties of Poly(manganese 1,1â€²-ferrocenediyl-bis(H-phosphinate)). Crystal Growth and Design, 2016, 16, 5084-5090.	3.0	34
35	FT-Raman, FT-IR spectroscopic and DFT studies of hexaphenoxycyclotriphosphazene. Journal of Molecular Structure, 2016, 1115, 124-135.	3.6	4
36	Comparative DFT study of structure, reactivity and IR spectra of phosphorus-containing dendrons with PNPS linkages, vinyl and azide functional groups. Journal of Molecular Structure, 2015, 1091, 6-15.	3.6	4

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37	Raman spectroscopy studies of phosphorus dendrimers with phenoxy and deuterophenoxy terminal groups. Vibrational Spectroscopy, 2015, 80, 17-23.	2.2	1
38	The key role of the scaffold on the efficiency of dendrimer nanodrugs. Nature Communications, 2015, 6, 7722.	12.8	133
39	DFT study of structure, IR and Raman spectra of dendrimer with PNPS linkages and its complexation with gold. Journal of Molecular Structure, 2015, 1084, 103-113.	3.6	6
40	Spectroscopic and molecular structure investigation of the phosphorus-containing Gâ€²2 dendrimer with terminal aldehyde groups using DFT method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 137, 220-226.	3.9	2
41	Stability of Isolated-Pentagon-Rule Isomers of Fullerene C₇₆. Fullerenes Nanotubes and Carbon Nanostructures, 2015, 23, 148-152.	2.1	13
42	Doping and Theory: general discussion. Faraday Discussions, 2014, 173, 233-256.	3.2	4
43	DFT study of Raman spectra of hexakis(4-Nâ€²(-di(4-oxyphenethylamino)-(thio)phosphonyl)-Nâ€²-methyl-diazobenzene)cyclotriphosphazene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 128, 212-217.	3.9	0
44	Electronic structures of some of C84 fullerene isomers and the structures of their perfluoroalkyl derivatives. Russian Journal of Physical Chemistry A, 2014, 88, 103-107.	0.6	4
45	Comparative DFT study of Raman spectra of phosphorus-containing dendrimers built from thiophosphoryl, cyclotriphosphazene and phthalocyanine cores. Vibrational Spectroscopy, 2014, 70, 78-88.	2.2	2
46	DFT study of structure, IR and Raman spectra of phosphorus-containing dendron with azide functional group. Vibrational Spectroscopy, 2014, 75, 1-10.	2.2	8
47	DFT study of Raman spectra of phosphorus-containing dendrons built from cyclotriphosphazene core with terminal carbamate and ester groups. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 195-200.	3.9	1
48	DFT study of the IR and Raman spectra of a fluorescent dendron built from cyclotriphosphazene core. Vibrational Spectroscopy, 2014, 73, 28-36.	2.2	0
49	Vibrational spectra study of phosphorus dendrimer containing azobenzene, ammonium and carbamate groups. Chemical Physics, 2013, 421, 57-67.	1.9	6
50	DFT study of Raman spectra of phosphorus-containing dendrons built from cyclotriphosphazene core. Journal of Molecular Structure, 2013, 1051, 197-204.	3.6	1
51	DFT study of Raman spectra of phosphorus-containing dendrimers built from thiophosphoryl core. Vibrational Spectroscopy, 2013, 68, 61-70.	2.2	0
52	Vibrational spectra study of phosphorus dendrimer containing azobenzene units on the surface. Journal of Molecular Structure, 2013, 1046, 30-38.	3.6	3
53	Structural and spectroscopic properties of the second generation phosphorusâ€“viologen â€œmolecular asteriskâ€• Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 115, 183-190.	3.9	2
54	DFT study of structure, IR and Raman spectra of the first generation dendrimer built from cyclotriphosphazene core with terminal 4-oxyphenethylamino groups. Journal of Molecular Structure, 2012, 1026, 17-22.	3.6	0

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55	Experimental vibrational spectra and computational study of 1,4-diazabicyclo[2.2.2]octane. Journal of Molecular Structure, 2012, 1028, 134-140.	3.6	23
56	IR and Raman spectra, hydrogen bonds, and conformations of N-(2-hydroxyethyl)-4,6-dimethyl-2-oxo-1,2-dihydropyrimidine (drug Xymedone). Russian Chemical Bulletin, 2012, 61, 1199-1206.	1.5	9
57	24 IPR isomers of fullerene C₈₄: Cage deformation as geometrical characteristic of local strains. International Journal of Quantum Chemistry, 2012, 112, 1055-1065.	2.0	9
58	DFT study of structure, IR and Raman spectra of the first generation dendron built from cyclotriphosphazene core with terminal carbamate and ester groups. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 91, 97-105.	3.9	2
59	Electronic Structure and Stability of Fullerene C₈₂ Isolated-Pentagon-Rule Isomers. Journal of Physical Chemistry A, 2011, 115, 12315-12320.	2.5	22
60	DFT study of structure, IR and Raman spectra of the fluorescent â€œJanusâ€•dendron built from cyclotriphosphazene core. Journal of Molecular Structure, 2011, 1005, 25-30.	3.6	7
61	Electronic Structure and Stability of C₈₀Fullerene IPR Isomers. Fullerenes Nanotubes and Carbon Nanostructures, 2011, 19, 599-604.	2.1	19
62	Vibrational spectra study of fluorescent dendrimers built from the cyclotriphosphazene core with terminal dansyl and carbamate groups. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 462-470.	3.9	8
63	Electronic structure and stability of C₈₆ fullerene Isolatedâ€Pentagonâ€Rule isomers. International Journal of Quantum Chemistry, 2011, 111, 2966-2971.	2.0	5
64	DFT study of structure, IR and Raman spectra of the first generation dendron built from cyclotriphosphazene core. Journal of Molecular Structure, 2011, 987, 144-151.	3.6	2
65	Specific vapor sorption properties of phosphorus-containing dendrimers. Journal of Colloid and Interface Science, 2011, 360, 204-210.	9.4	11
66	Raman spectroscopy study of phosphorus-containing dendrimers built from thiophosphoryl core. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 76, 276-282.	3.9	3
67	Vibrational spectroscopy studies of dendrimers built from cyclophosphazene core with terminal oxybenzaldehyde groups. Journal of Molecular Structure, 2010, 971, 62-70.	3.6	2
68	DFT calculations of structure and vibrational spectra of dendron built of cyclotriphosphazene core with terminal carbamate and ester groups. Vibrational Spectroscopy, 2010, 54, 21-29.	2.2	4
69	Crystalline cellulose: structure and hydrogen bonds. Russian Chemical Reviews, 2010, 79, 231-241.	6.5	66
70	IR spectroscopy and DFT study of phosphorus-containing G2 generation dendrimer. Journal of Molecular Structure, 2009, 919, 366-372.	3.6	17
71	Comparative IR spectroscopic study of phosphorus-containing dendrimers built of thiophosphoryl, cyclophosphazene and phthalocyanine cores. Vibrational Spectroscopy, 2009, 51, 326-332.	2.2	2
72	DFT analysis of vibrational spectra of phosphorus-containing dendrons built from cyclotriphosphazene core. Journal of Molecular Structure, 2009, 932, 97-104.	3.6	8

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73	IR spectroscopy investigation using DFT analysis on the structure of P1 phosphorus dendrimer built from octasubstituted metal-free phthalocyanine core. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2009, 72, 636-642.	3.9	1
74	DFT study of structure, IR and Raman spectra of and dendrimers built from octasubstituted metal-free phthalocyanine core. Chemical Physics, 2009, 358, 177-183.	1.9	19
75	Unusual pentagon and hexagon geometry of three isomers (no 1, 20, and 23) of fullerene C₈₄. International Journal of Quantum Chemistry, 2008, 108, 1334-1339.	2.0	19
76	Molecular structure and IR spectra of generation phosphorus dendrimer built from cyclophosphazene core with terminal phenoxy groups by DFT calculations. Journal of Molecular Structure, 2008, 886, 1-8.	3.6	8
77	FTIR spectroscopy and DFT studies of carbosilane dendrimers. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 70, 692-699.	3.9	6
78	FTIR and FT-Raman spectra and DFT vibrational analysis of phosphorus-containing dendrons. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1110-1118.	3.9	2
79	DFT study of the structure and IR spectra of Gc1 model compound built from cyclotriphosphazene core. Journal of Molecular Structure, 2008, 875, 587-593.	3.6	20
80	Stability of the Nonâ€IPR Isomers 6140 (D₃) and 6275 (D₃) of Fullerene C₆₈. Fullerenes Nanotubes and Carbon Nanostructures, 2008, 16, 542-545.	2.1	9
81	Spectral additive properties of phosphorus-containing dendrimers. Vibrational Spectroscopy, 2007, 43, 351-357.	2.2	6
82	FTIR spectroscopy studies of dendrimers built from cyclophosphazene core. Vibrational Spectroscopy, 2007, 44, 89-93.	2.2	4
83	DFT analysis of structure and IR spectra of phosphorus G1v generation dendron. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 66, 745-753.	3.9	5
84	ELECTRONIC STRUCTURE AND STABILITY OF HIGHER FULLERENES. , 2007, , 437-441.		5
85	DFT study and vibrational spectra of the phoshorus-containing G0 generation dendrimer. Vibrational Spectroscopy, 2006, 40, 155-160.	2.2	14
86	DFT study and IR spectra of hexaphenoxycyclotriphosphazene generation phosphorus dendrimer. Chemical Physics, 2006, 330, 349-354.	1.9	5
87	DFT study and IR spectra of the phosphorus-containing G1 generation dendrimer. Journal of Molecular Structure, 2006, 785, 133-138.	3.6	12
88	Modelling conformations and IR spectra of p-tert-butylthiacalix[4]arene tetraester using DFT method. Journal of Molecular Structure, 2006, 825, 38-44.	3.6	9
89	DFT and IR spectroscopic analysis of p-tert-butylthiacalix[4]arene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 63, 207-212.	3.9	29
90	DFT calculations of structure and IR spectra of the phoshorus-containing Gâ€²0v generation dendron. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 358-365.	3.9	5

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91	DFT calculation of molecular structure and vibrational spectra of the phosphorus-containing generation dendrimer with terminal aldehyde groups. Chemical Physics, 2006, 326, 417-424.	1.9	20
92	Band intensity in the IR spectra and conformations of calix[4]arene and thiacalix[4]arene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 355-359.	3.9	33
93	The hydrogen bonding and conformations of p-tert-butylcalix[4]arene as studied by IR spectroscopy and by DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 483-493.	3.9	35
94	Vibrational spectra, co-operative intramolecular hydrogen bonding and conformations of calix[4]arene and thiacalix[4]arene molecules and their para-tert-butyl derivatives. Organic and Biomolecular Chemistry, 2005, 3, 2558.	2.8	41
95	Elementoorganic dendrimer characterization by Raman spectroscopy. Polymer, 2004, 45, 5889-5895.	3.8	7
96	Fourier-transform infrared and Raman difference spectroscopy studies of the phosphorus-containing dendrimers. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 1649-1657.	3.9	15
97	Open-shell fullerene C74: phenalenyl-radical substructures. Chemical Physics Letters, 2003, 377, 263-268.	2.6	54
98	The vibrational analysis of the starting â€œmonomerâ€•and first generation of the starburst elementoorganic dendrimer. Vibrational Spectroscopy, 2003, 31, 71-79.	2.2	20
99	Calculation of IR spectra of the elementoorganic dendrimers. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 2905-2912.	3.9	14
100	The vibrational spectra of the elementoorganic starburst dendrimers. Journal of Molecular Structure, 2002, 604, 45-56.	3.6	38
101	A 13C NMR study of cellulose nitrates. Polymer Science USSR, 1987, 29, 1111-1117.	0.2	3
102	Structural changes in cellulose caused by the action of dichloromethane. Polymer Science USSR, 1983, 25, 1647-1652.	0.2	2
103	Relation between the crystalline structure and molecular weight of polyethylene adipate. Polymer Science USSR, 1976, 18, 1596-1604.	0.2	3
104	Kinetics of three dimensional radical polymerization of butadiene phosphinates. Polymer Science USSR, 1974, 16, 1599-1606.	0.2	0
105	Phosphorus-containing mixed polyamides based on carboxyl derivatives of phosphinic acid. Polymer Science USSR, 1971, 13, 2673-2681.	0.2	0
106	Diethylphosphonacetals of polyvinyl alcohol. Polymer Science USSR, 1970, 12, 646-652.	0.2	3
107	Polymorphism in poly (Ethylene glycol adipate). Polymer Science USSR, 1967, 9, 1880-1888.	0.2	15
108	Features of molecular structures of some IPR isomers of C96 fullerene. Structural Chemistry, 0, , 1.	2.0	0