

# Valeri I Kovalenko

## List of Publications by Year in descending order

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108  
papers

1,161  
citations

430874

18  
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477307

29  
g-index

108  
all docs

108  
docs citations

108  
times ranked

1149  
citing authors

#	ARTICLE	IF	CITATIONS
1	The key role of the scaffold on the efficiency of dendrimer nanodrugs. <i>Nature Communications</i> , 2015, 6, 7722.	12.8	133
2	Crystalline cellulose: structure and hydrogen bonds. <i>Russian Chemical Reviews</i> , 2010, 79, 231-241.	6.5	66
3	Open-shell fullerene C74: phenalenyl-radical substructures. <i>Chemical Physics Letters</i> , 2003, 377, 263-268.	2.6	54
4	Vibrational spectra, co-operative intramolecular hydrogen bonding and conformations of calix[4]arene and thiacalix[4]arene molecules and their para-tert-butyl derivatives. <i>Organic and Biomolecular Chemistry</i> , 2005, 3, 2558.	2.8	41
5	Zn and Co redox active coordination polymers as efficient electrocatalysts. <i>Dalton Transactions</i> , 2019, 48, 3601-3609.	3.3	41
6	The vibrational spectra of the elementoorganic starburst dendrimers. <i>Journal of Molecular Structure</i> , 2002, 604, 45-56.	3.6	38
7	The hydrogen bonding and conformations of p-tert-butylcalix[4]arene as studied by IR spectroscopy and by DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 62, 483-493.	3.9	35
8	Reversible Water-Induced Structural and Magnetic Transformations and Selective Water Adsorption Properties of Poly(manganese 1,1'-ferrocenediyl-bis(H-phosphinate)). <i>Crystal Growth and Design</i> , 2016, 16, 5084-5090.	3.0	34
9	Band intensity in the IR spectra and conformations of calix[4]arene and thiacalix[4]arene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2005, 61, 355-359.	3.9	33
10	DFT and IR spectroscopic analysis of p-tert-butylthiacalix[4]arene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 63, 207-212.	3.9	29
11	DFT study of hydrogen bonding and IR spectra of calix[6]arene. <i>Journal of Molecular Structure</i> , 2017, 1128, 439-447.	3.6	24
12	Experimental vibrational spectra and computational study of 1,4-diazabicyclo[2.2.2]octane. <i>Journal of Molecular Structure</i> , 2012, 1028, 134-140.	3.6	23
13	Electronic Structure and Stability of Fullerene C <sub>82</sub> Isolated-Pentagon-Rule Isomers. <i>Journal of Physical Chemistry A</i> , 2011, 115, 12315-12320.	2.5	22
14	The vibrational analysis of the starting monomer and first generation of the starburst elementoorganic dendrimer. <i>Vibrational Spectroscopy</i> , 2003, 31, 71-79.	2.2	20
15	DFT calculation of molecular structure and vibrational spectra of the phosphorus-containing generation dendrimer with terminal aldehyde groups. <i>Chemical Physics</i> , 2006, 326, 417-424.	1.9	20
16	DFT study of the structure and IR spectra of Gc1 model compound built from cyclotriphosphazene core. <i>Journal of Molecular Structure</i> , 2008, 875, 587-593.	3.6	20
17	FT-IR and FT-Raman study of hydrogen bonding in p-alkylcalix[8]arenes. <i>Vibrational Spectroscopy</i> , 2018, 95, 38-43.	2.2	20
18	Unusual pentagon and hexagon geometry of three isomers (no 1, 20, and 23) of fullerene C <sub>84</sub> . <i>International Journal of Quantum Chemistry</i> , 2008, 108, 1334-1339.	2.0	19

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19	DFT study of structure, IR and Raman spectra of and dendrimers built from octasubstituted metal-free phthalocyanine core. <i>Chemical Physics</i> , 2009, 358, 177-183.	1.9	19
20	Electronic Structure and Stability of C <sub>80</sub> Fullerene IPR Isomers. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2011, 19, 599-604.	2.1	19
21	IR spectroscopy and DFT study of phosphorus-containing G2 generation dendrimer. <i>Journal of Molecular Structure</i> , 2009, 919, 366-372.	3.6	17
22	Polymorphism in poly (Ethylene glycol adipate). <i>Polymer Science USSR</i> , 1967, 9, 1880-1888.	0.2	15
23	Fourier-transform infrared and Raman difference spectroscopy studies of the phosphorus-containing dendrimers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2004, 60, 1649-1657.	3.9	15
24	Calculation of IR spectra of the elementoorganic dendrimers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2002, 58, 2905-2912.	3.9	14
25	DFT study and vibrational spectra of the phoshorus-containing G0 generation dendrimer. <i>Vibrational Spectroscopy</i> , 2006, 40, 155-160.	2.2	14
26	IR and UV study of reversible water-induced structural transformations of poly(manganese) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 467 To of <i>Molecular Structure</i> , 2018, 1166, 237-242.	3.6	14
27	Stability of Isolated-Pentagon-Rule Isomers of Fullerene C <sub>76</sub> . <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2015, 23, 148-152.	2.1	13
28	In silico exploration of O-Hâ€¦X <sub>2</sub> (X=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. <i>Journal of Molecular Liquids</i> , 2021, 334, 116127.	4.9	13
29	DFT study and IR spectra of the phosphorus-containing G1 generation dendrimer. <i>Journal of Molecular Structure</i> , 2006, 785, 133-138.	3.6	12
30	Specific vapor sorption properties of phosphorus-containing dendrimers. <i>Journal of Colloid and Interface Science</i> , 2011, 360, 204-210.	9.4	11
31	Substructural Approach for Assessing the Stability of Higher Fullerenes. <i>International Journal of Molecular Sciences</i> , 2021, 22, 3760.	4.1	10
32	Modelling conformations and IR spectra of p-tert-butylthiacalix[4]arene tetraester using DFT method. <i>Journal of Molecular Structure</i> , 2006, 825, 38-44.	3.6	9
33	Stability of the Nonâ€¦IPR Isomers 6140 (D <sub>3</sub> ) and 6275 (D <sub>3</sub> ) of Fullerene C <sub>68</sub> . <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2008, 16, 542-545.	2.1	9
34	IR and Raman spectra, hydrogen bonds, and conformations of N-(2-hydroxyethyl)-4,6-dimethyl-2-oxo-1,2-dihydropyrimidine (drug Xymedone). <i>Russian Chemical Bulletin</i> , 2012, 61, 1199-1206.	1.5	9
35	24 IPR isomers of fullerene C <sub>84</sub> : Cage deformation as geometrical characteristic of local strains. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 1055-1065.	2.0	9
36	Cyclic cooperative intramolecular hydrogen bond in p-tert-butylcalix[6]arene according to FTIR spectroscopy and DFT studies. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2017, 181, 98-108.	3.9	9

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37	Investigation of hydrogen bonding in p-sulfonatocalix[4]arene and its thermal stability by vibrational spectroscopy. <i>Journal of Molecular Structure</i> , 2019, 1195, 403-410.	3.6	9
38	Vibrational spectra study of p-sulfonatocalix[4]arene containing azobenzene groups. <i>Journal of Molecular Structure</i> , 2020, 1200, 127058.	3.6	9
39	Molecular structure and IR spectra of generation phosphorus dendrimer built from cyclophosphazene core with terminal phenoxy groups by DFT calculations. <i>Journal of Molecular Structure</i> , 2008, 886, 1-8.	3.6	8
40	DFT analysis of vibrational spectra of phosphorus-containing dendrons built from cyclotriphosphazene core. <i>Journal of Molecular Structure</i> , 2009, 932, 97-104.	3.6	8
41	Vibrational spectra study of fluorescent dendrimers built from the cyclotriphosphazene core with terminal dansyl and carbamate groups. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 79, 462-470.	3.9	8
42	DFT study of structure, IR and Raman spectra of phosphorus-containing dendron with azide functional group. <i>Vibrational Spectroscopy</i> , 2014, 75, 1-10.	2.2	8
43	Structure, IR and Raman spectra of phosphotrihydrazide studied by DFT. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 166, 19-24.	3.9	8
44	Radical IPR Fullerenes C <sub>74</sub> (D <sub>3h</sub> ) and C <sub>76</sub> (T <sub>d</sub> ): Dimer, Trimer, etc. <i>Experiments and Theory. Journal of Physical Chemistry C</i> , 2018, 122, 3146-3151.	3.1	8
45	FT-IR and FT-Raman study of p-sulfonatocalix [8]arene. <i>Journal of Molecular Structure</i> , 2020, 1203, 127474.	3.6	8
46	Elementoorganic dendrimer characterization by Raman spectroscopy. <i>Polymer</i> , 2004, 45, 5889-5895.	3.8	7
47	DFT study of structure, IR and Raman spectra of the fluorescent $\alpha$ -Janus-dendron built from cyclotriphosphazene core. <i>Journal of Molecular Structure</i> , 2011, 1005, 25-30.	3.6	7
48	Spectral additive properties of phosphorus-containing dendrimers. <i>Vibrational Spectroscopy</i> , 2007, 43, 351-357.	2.2	6
49	FTIR spectroscopy and DFT studies of carbosilane dendrimers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 70, 692-699.	3.9	6
50	Vibrational spectra study of phosphorus dendrimer containing azobenzene, ammonium and carbamate groups. <i>Chemical Physics</i> , 2013, 421, 57-67.	1.9	6
51	DFT study of structure, IR and Raman spectra of dendrimer with PNPS linkages and its complexation with gold. <i>Journal of Molecular Structure</i> , 2015, 1084, 103-113.	3.6	6
52	Ythrene: From the Real Radical Fullerene Substructure to Hypothetical (yet?) Radical Molecules. <i>Journal of Physical Chemistry C</i> , 2019, 123, 1954-1959.	3.1	6
53	Features of molecular structure of small non-IPR fullerenes: the two isomers of C <sub>50</sub> . <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	1.4	6
54	DFT study and IR spectra of hexaphenoxycyclotriphosphazene generation phosphorus dendrimer. <i>Chemical Physics</i> , 2006, 330, 349-354.	1.9	5

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55	DFT calculations of structure and IR spectra of the phosphorus-containing G <sub>0</sub> generation dendron. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2006, 65, 358-365.	3.9	5
56	DFT analysis of structure and IR spectra of phosphorus G <sub>1</sub> generation dendron. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2007, 66, 745-753.	3.9	5
57	Electronic structure and stability of C <sub>86</sub> fullerene Isolated $\Delta$ -Pentagon $\Delta$ -Rule isomers. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 2966-2971.	2.0	5
58	Stabilization of IPR open-shell fullerenes C <sub>74</sub> (D <sub>3h</sub> ) and C <sub>76</sub> (T <sub>d</sub> ) in radical addition reactions. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2017, 25, 128-132.	2.1	5
59	Investigation of the conformation and hydrogen bonds in adamantylthiacalix[4]arene by IR spectroscopy and DFT. <i>Journal of Molecular Structure</i> , 2018, 1171, 207-213.	3.6	5
60	DFT study of conformation, hydrogen bonds, IR, and Raman spectra of the sodium salt of p-hexasulfonatocalix[6]arene DFT. <i>Journal of Molecular Structure</i> , 2021, 1243, 130892.	3.6	5
61	Open-shell nature of non-IPR fullerene $\Delta$ <sub>140</sub> : isomers 29 (C <sub>2</sub> ) and 40 (T <sub>d</sub> ). <i>Journal of Molecular Modeling</i> , 2021, 27, 22.	1.8	5
62	ELECTRONIC STRUCTURE AND STABILITY OF HIGHER FULLERENES. , 2007, , 437-441.		5
63	FTIR spectroscopy studies of dendrimers built from cyclophosphazene core. <i>Vibrational Spectroscopy</i> , 2007, 44, 89-93.	2.2	4
64	DFT calculations of structure and vibrational spectra of dendron built of cyclotriphosphazene core with terminal carbamate and ester groups. <i>Vibrational Spectroscopy</i> , 2010, 54, 21-29.	2.2	4
65	Doping and Theory: general discussion. <i>Faraday Discussions</i> , 2014, 173, 233-256.	3.2	4
66	Electronic structures of some of C <sub>84</sub> fullerene isomers and the structures of their perfluoroalkyl derivatives. <i>Russian Journal of Physical Chemistry A</i> , 2014, 88, 103-107.	0.6	4
67	Comparative DFT study of structure, reactivity and IR spectra of phosphorus-containing dendrons with PNPS linkages, vinyl and azide functional groups. <i>Journal of Molecular Structure</i> , 2015, 1091, 6-15.	3.6	4
68	FT-Raman, FT-IR spectroscopic and DFT studies of hexaphenoxycyclotriphosphazene. <i>Journal of Molecular Structure</i> , 2016, 1115, 124-135.	3.6	4
69	Molecular structures of the open-shell IPR isomers of fullerene C <sub>90</sub> . <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2017, 25, 179-184.	2.1	4
70	DFT study of structure, IR and Raman spectra of the first generation dendrimer built from cyclotriphosphazene core with terminal pyrazine groups. <i>Vibrational Spectroscopy</i> , 2017, 92, 54-61.	2.2	4
71	The key feature of instability of small non-IPR closed-shell fullerenes: three isomers of C <sub>40</sub> . <i>Mendeleev Communications</i> , 2020, 30, 725-727.	1.6	4
72	Diethylphosphonacetals of polyvinyl alcohol. <i>Polymer Science USSR</i> , 1970, 12, 646-652.	0.2	3

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73	Relation between the crystalline structure and molecular weight of polyethylene adipate. <i>Polymer Science USSR</i> , 1976, 18, 1596-1604.	0.2	3
74	A <sup>13</sup> C NMR study of cellulose nitrates. <i>Polymer Science USSR</i> , 1987, 29, 1111-1117.	0.2	3
75	Raman spectroscopy study of phosphorus-containing dendrimers built from thiophosphoryl core. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 76, 276-282.	3.9	3
76	Vibrational spectra study of phosphorus dendrimer containing azobenzene units on the surface. <i>Journal of Molecular Structure</i> , 2013, 1046, 30-38.	3.6	3
77	Synthesis and study of the vibrational spectra of a first generation phosphorus-containing dendrimer with pyridyl functional groups. <i>Journal of Molecular Structure</i> , 2018, 1162, 1-9.	3.6	3
78	Vibrational spectroscopic investigation of the gold complexation within the cascade structure of phosphorus-containing dendrimer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 203, 118-126.	3.9	3
79	Structural changes in cellulose caused by the action of dichloromethane. <i>Polymer Science USSR</i> , 1983, 25, 1647-1652.	0.2	2
80	FTIR and FT-Raman spectra and DFT vibrational analysis of phosphorus-containing dendrons. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008, 71, 1110-1118.	3.9	2
81	Comparative IR spectroscopic study of phosphorus-containing dendrimers built of thiophosphoryl, cyclophosphazene and phthalocyanine cores. <i>Vibrational Spectroscopy</i> , 2009, 51, 326-332.	2.2	2
82	Vibrational spectroscopy studies of dendrimers built from cyclophosphazene core with terminal oxybenzaldehyde groups. <i>Journal of Molecular Structure</i> , 2010, 971, 62-70.	3.6	2
83	DFT study of structure, IR and Raman spectra of the first generation dendron built from cyclotriphosphazene core. <i>Journal of Molecular Structure</i> , 2011, 987, 144-151.	3.6	2
84	DFT study of structure, IR and Raman spectra of the first generation dendron built from cyclotriphosphazene core with terminal carbamate and ester groups. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 91, 97-105.	3.9	2
85	Structural and spectroscopic properties of the second generation phosphorus- <sup>viologen</sup> molecular asterisk. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 115, 183-190.	3.9	2
86	Comparative DFT study of Raman spectra of phosphorus-containing dendrimers built from thiophosphoryl, cyclotriphosphazene and phthalocyanine cores. <i>Vibrational Spectroscopy</i> , 2014, 70, 78-88.	2.2	2
87	Spectroscopic and molecular structure investigation of the phosphorus-containing C <sup>2</sup> dendrimer with terminal aldehyde groups using DFT method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 137, 220-226.	3.9	2
88	DFT study of IR and Raman spectra of phosphotrihydrazone dendrimer with terminal phenolic groups. <i>Journal of Molecular Structure</i> , 2017, 1144, 466-472.	3.6	2
89	Vibrational spectra and DFT studies of conjugation in poly(phosphorhydrazone) dendrimers. <i>Vibrational Spectroscopy</i> , 2017, 88, 14-26.	2.2	2
90	Vibrational spectroscopic study of cationic phosphorus dendrimers with aminoethylpiperidine terminal groups. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 194, 211-221.	3.9	2

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91	IR spectroscopy investigation using DFT analysis on the structure of P1 phosphorus dendrimer built from octasubstituted metal-free phthalocyanine core. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2009, 72, 636-642.	3.9	1
92	DFT study of Raman spectra of phosphorus-containing dendrons built from cyclotriphosphazene core. <i>Journal of Molecular Structure</i> , 2013, 1051, 197-204.	3.6	1
93	DFT study of Raman spectra of phosphorus-containing dendrons built from cyclotriphosphazene core with terminal carbamate and ester groups. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 120, 195-200.	3.9	1
94	Raman spectroscopy studies of phosphorus dendrimers with phenoxy and deuterophenoxy terminal groups. <i>Vibrational Spectroscopy</i> , 2015, 80, 17-23.	2.2	1
95	Vibrational spectroscopic study on polycationic phosphorus dendrimers. <i>Vibrational Spectroscopy</i> , 2017, 93, 65-77.	2.2	1
96	Radical character of non-IPR isomer 17418 (C1) of fullerene C76. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2021, 29, 678-684.	2.1	1
97	Comparative study of the vibrational spectra of carboxylate azocalix[4]arenes and azothiocalix[4]arenes. <i>Journal of Molecular Structure</i> , 2021, 1241, 130662.	3.6	1
98	Investigation of H-bonding of p-(3-carboxymethyl-1-adamantyl)calix[6]arene by IR spectroscopy. <i>Journal of Molecular Structure</i> , 2022, 1248, 131472.	3.6	1
99	Phosphorus-containing mixed polyamides based on carboxyl derivatives of phosphinic acid. <i>Polymer Science USSR</i> , 1971, 13, 2673-2681.	0.2	0
100	Kinetics of three dimensional radical polymerization of butadiene phosphinates. <i>Polymer Science USSR</i> , 1974, 16, 1599-1606.	0.2	0
101	DFT study of structure, IR and Raman spectra of the first generation dendrimer built from cyclotriphosphazene core with terminal 4-oxyphenethylamino groups. <i>Journal of Molecular Structure</i> , 2012, 1026, 17-22.	3.6	0
102	DFT study of Raman spectra of phosphorus-containing dendrimers built from thiophosphoryl core. <i>Vibrational Spectroscopy</i> , 2013, 68, 61-70.	2.2	0
103	DFT study of Raman spectra of hexakis(4-Na <sup>+</sup> -di(4-oxyphenethylamino)-(thio)phosphonyl)-N <sup>+</sup> -methyl-diazobenzene)cyclotriphosphazene. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 128, 212-217.	3.9	0
104	DFT study of the IR and Raman spectra of a fluorescent dendron built from cyclotriphosphazene core. <i>Vibrational Spectroscopy</i> , 2014, 73, 28-36.	2.2	0
105	Investigation of the structure and hydrogen bonds in adamantylcalix[6]arene by IR spectroscopy and DFT. <i>Vibrational Spectroscopy</i> , 2018, 96, 60-66.	2.2	0
106	Fullerenes C100 and C108: new substructures of higher fullerenes. <i>Structural Chemistry</i> , 2021, 32, 2283-2290.	2.0	0
107	Features of molecular structures of some IPR isomers of C96 fullerene. <i>Structural Chemistry</i> , 0, , 1.	2.0	0
108	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. <i>Journal of Molecular Structure</i> , 2021, 1239, 130508.	3.6	0