Juan JesÃºs LÃ³pez GonzÃ¡lez

List of Publications by Year
in descending order

126 papers	1,847 citations	304743 22 h-index	377865 34 g-index
128 all docs	128 docs citations	128 times ranked	1765 citing authors

#	Article	IF	Citations
1	A new insight into the vibrational analysis of pyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 2815-2839.	3.9	121
2	Photoinduced Chiral Nematic Organization in an Achiral Glassy Nematic Azopolymer. Advanced Functional Materials, 2007, 17, 3486-3492.	14.9	82
3	Theoretical and experimental vibrational spectrum study of 4-hydroxybenzoic acid as monomer and dimer. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 1422-1434.	3.9	59
4	Intermolecular Charge Transfer and Hydrogen Bonding in Solid Furan. Journal of the American Chemical Society, 2004, 126, 15087-15095.	13.7	54
5	Measurement and ab initio modeling of the inelastic neutron scattering of solid melamine. Chemical Physics, 2001, 266, 1-17.	1.9	50
6	Conformational relaxation of S-(+)-carvone and R-(+)-limonene studied by microwave Fourier transform spectroscopy and quantum chemical calculations. Structural Chemistry, 2013, 24, 1163-1170.	2.0	50
7	Conformational study of (R)-(+)-limonene in the liquid phase using vibrational spectroscopy (IR,) Tj ETQq1 1 0.784314 rgBT /Overlock	1.8	47
8	Synthesis and vibrational analysis of Nâ€(2â€²â€Furyl)â€imidazole. Journal of Raman Spectroscopy, 2009, 40, 1004-1010.	2.5	40
9	Conformational Flexibility in Terpenes: Vibrational Circular Dichroism (VCD), Infrared and Raman Study of S-(â˜)-Perillaldehyde. Journal of Physical Chemistry A, 2008, 112, 7887-7893.	2.5	38
10	Structural and vibrational study of 2â€(2â€²â€furyl)â€1Hâ€imidazole. Journal of Physical Organic Chemistry, 2008, 21, 1086-1097.	1.9	34
11	Structural and vibrational analyses of 2â€(2â€benzofuranyl)â€2â€imidazoline. Journal of Raman Spectroscopy, 2011, 42, 108-116.	2.5	33
12	The chiral structure of 1H-indazoles in the solid state: a crystallographic, vibrational circular dichroism and computational study. New Journal of Chemistry, 2012, 36, 749.	2.8	32
13	Conformational landscape in chiral terpenes from vibrational spectroscopy and quantum chemical calculations: S-(+)-carvone. Vibrational Spectroscopy, 2009, 51, 318-325.	2.2	31
14	Chiral Recognition of Amino Acid Enantiomers by a Crown Ether: Chiroptical IR-VCD Response and Computational Study. Journal of Physical Chemistry B, 2013, 117, 9362-9370.	2.6	31
15	Vibrational spectra of trimethylsilanol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 1169-1178.	3.9	26
16	Vibrational analysis of the inelastic neutron scattering spectrum of s-triazine and trichloro-s-triazine. Chemical Physics, 1995, 200, 395-403.	1.9	25
17	Unambiguous formalism of molecular vibrations: Use of redundant coordinates and canonical matrices. Journal of Chemical Physics, 1999, 110, 3302-3308.	3.0	25
18	Inelastic Neutron Scattering Spectrum and Quantum Mechanical Calculations on the Internal Vibrations of Pyrimidine. Journal of Physical Chemistry A, 1999, 103, 5833-5840.	2.5	25

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19	Structural and vibrational study of 2â€(2â€²â€•furyl)â€4,5â€1 Hâ€dihydroimidazole. Journal of Physical Organic Chemistry, 2009, 22, 1166-1177.	1.9	25
20	IRâ€“Ramanâ€“VCD study of R-(+)-Pulegone: Influence of the solvent. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 767-776.	3.9	24
21	Structural and vibrational study of 4-(2â€²-furyl)-1-methylimidazole. Journal of Molecular Structure, 2009, 924-926, 322-331.	3.6	23
22	Conformational preference of short aromatic amino acids from the FT-IR, FT-Raman and Far-IR spectroscopies, and quantum chemical calculations: l-phenylalanine and l-tyrosine. Tetrahedron: Asymmetry, 2012, 23, 1084-1092.	1.8	23
23	l-Serine in aqueous solutions at different pH: Conformational preferences and vibrational spectra of cationic, anionic and zwitterionic species. Journal of Molecular Structure, 2013, 1046, 136-146.	3.6	23
24	Carbohydrates in the gas phase: conformational preference ofd-ribose and 2-deoxy-d-ribose. New Journal of Chemistry, 2014, 38, 529-538.	2.8	23
25	A topological geometric method for the obtention of symmetry-adapted functions for point groups III. The cubic group. Computers and Mathematics With Applications, 1995, 29, 35-39.	2.7	21
26	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.	2.5	21
27	Terpenes in the gas phase: The structural conformation of S-(â€“)-perillaldehyde investigated by microwave spectroscopy and quantum chemical calculations. Chemical Physics Letters, 2009, 473, 17-20.	2.6	21
28	Conformational preference of a chiral terpene: vibrational circular dichroism (VCD), infrared and Raman study of S-(â˜)-limonene oxide. Physical Chemistry Chemical Physics, 2009, 11, 2459.	2.8	21
29	Experimental and ab Initio Equilibrium Structure and Harmonic Force Field of 1,2,5-Oxadiazole. Journal of Molecular Spectroscopy, 2001, 207, 224-237.	1.2	20
30	Vibrational spectra and structure of methoxysilanes and products of their hydrolysis. Vibrational Spectroscopy, 2006, 40, 1-9.	2.2	19
31	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.	2.5	19
32	A vibrational circular dichroism (VCD) methodology for the measurement of enantiomeric excess in chiral compounds in the solid phase and for the complementary use of NMR and VCD techniques in solution: the camphor case. Analyst, The, 2018, 143, 1406-1416.	3.5	19
33	Study of the Photoinduced Supramolecular Chirality in Columnar Liquid Crystals by Infrared and VCD Spectroscopies. Journal of Physical Chemistry B, 2012, 116, 5090-5096.	2.6	18
34	Supramolecular organization of perfluorinated 1H-indazoles in the solid state using X-ray crystallography, SSNMR and sensitive (VCD) and non sensitive (MIR, FIR and Raman) to chirality vibrational spectroscopies. Physical Chemistry Chemical Physics, 2017, 19, 1632-1643.	2.8	18
35	Theoretical study of the mechanisms of the hydrolysis and condensation reactions of silicon and titanium alkoxides: similarities and differences. Dalton Transactions, 2010, 39, 6967.	3.3	17
36	Conformational Preference and Chiroptical Response of Carbohydrates d-Ribose and 2-Deoxy-d-ribose in Aqueous and Solid Phases. Journal of Physical Chemistry B, 2013, 117, 14599-14614.	2.6	17

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37	Conformational landscape of l-threonine in neutral, acid and basic solutions from vibrational circular dichroism spectroscopy and quantum chemical calculations. Tetrahedron: Asymmetry, 2013, 24, 1537-1547.	1.8	17
38	Intramolecular hydrogen bonding in silanediols. Computational and Theoretical Chemistry, 2004, 678, 249-256.	1.5	16
39	Hydrogen bonding and structure of silanediol dimers and tetramers. Chemical Physics Letters, 2004, 384, 326-331.	2.6	16
40	Experimental and theoretical study of the hydration of phosphate groups in esters of biological interest. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 66, 884-897.	3.9	16
41	Structural, vibrational spectra and normal coordinate analysis for two tautomers of 4(5)â€(2â€²â€furyl)â€imidazole. Journal of Raman Spectroscopy, 2010, 41, 587-597.	2.5	15
42	Conformational Flexibility of Limonene Oxide Studied By Microwave Spectroscopy. ChemPhysChem, 2017, 18, 274-280.	2.1	15
43	Terpenes in the gas phase: The Far-IR spectrum of perillaldehyde. Journal of Quantitative Spectroscopy and Radiative Transfer, 2012, 113, 1261-1265.	2.3	14
44	Selfâ€Assembly Structures of 1 H â€indazoles in the Solution and Solid Phases: A Vibrational (IR, FIR,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.1	14
45	The Curious Case of 2-Propyl-1H-benzimidazole in the Solid State: An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2017, 121, 5665-5674.	2.5	14
46	Vibrational analysis of the inelastic neutron scattering spectrum of pyridine. Chemical Physics, 2000, 261, 239-247.	1.9	13
47	Experimental and Theoretical Analysis of the Vibrational Spectra and Theoretical Study of the Structures of 3,6-Dichloropyridazine and 3,4,5-Trichloropyridazine. Journal of Physical Chemistry A, 2000, 104, 2599-2612.	2.5	13
48	Condensation reactions in silanolâ€“water clusters. Chemical Physics Letters, 2003, 368, 616-624.	2.6	13
49	Vibrational spectrum of methoxytrimethylsilane. Journal of Molecular Structure, 2005, 744-747, 331-338.	3.6	13
50	Chiral self-assembly of enantiomerically pure (4S,7R)-campho[2,3-c]pyrazole in the solid state: a vibrational circular dichroism (VCD) and computational study. Tetrahedron: Asymmetry, 2014, 25, 507-515.	1.8	13
51	Structure Determination, Conformational Flexibility, Internal Dynamics, and Chiral Analysis of Pulegone and Its Complex with Water. Chemistry - A European Journal, 2018, 24, 721-729.	3.3	13
52	Transferability and Physicochemical Interpretation of Canonical Force Fields in Redundant Internal Coordinates:Â Pyridazine and 3,6-Dichloropyridazine. Journal of Physical Chemistry A, 2001, 105, 9354-9365.	2.5	12
53	Vibrational spectrum of chlorotrimethylsilane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 293-301.	3.9	12
54	Chiral terpenes in different phases: R-(â^')-camphorquinone studied by IRâ€“Ramanâ€“VCD spectroscopies and theoretical calculations. Structural Chemistry, 2011, 22, 67-76.	2.0	12

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55	Vibrational Circular Dichroism and Theoretical Study of the Conformational Equilibrium in (â^')â€‹Sâ€‹Nicotine. ChemPhysChem, 2015, 16, 342-352.	2.1	12
56	Calculation of internal valence force constants for XY4 (Td) tetrahedral molecules. Journal of Molecular Structure, 1992, 271, 237-249.	3.6	11
57	Weak Câ€“Hâ‹¯O and Câ€“Hâ‹¯Ï€ hydrogen bonds in crystal 1-indanone. An structural and spectroscopic analysis. Journal of Molecular Structure, 2004, 707, 33-46.	3.6	11
58	The vibrational spectra of (CH3)3SiX (S=H, F, Br) molecules, revisited. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 1058-1069.	3.9	11
59	Weak hydrogen-, halogen- and stacking Ï€â‹¯Ï€ bonding in crystalline 5-chloro-1-indanone. An analysis by using X-ray diffraction, vibrational spectroscopy and theoretical methods. Chemical Physics, 2006, 320, 164-180.	1.9	11
60	Structure and vibrational spectra of vinyl ether conformers. The comparison of B3LYP and MP2 predictions. Chemical Physics, 2007, 333, 148-156.	1.9	11
61	Conformational landscape of a chiral crown ether: a vibrational circular dichroism spectroscopy and computational study. Tetrahedron: Asymmetry, 2012, 23, 294-299.	1.8	11
62	Hydrogen bonding network in a chiral alcohol: (1R,2S,5R)-(â^')-menthol. Conformational preference studied by IRâ€“Ramanâ€“VCD spectroscopies and quantum chemical calculations. Structural Chemistry, 2013, 24, 671-680.	2.0	11
63	A Spectroscopic Study of Colchicine in the Solid State and in Solution by Multinuclear Magnetic Resonance and Vibrational Circular Dichroism. Helvetica Chimica Acta, 2014, 97, 471-490.	1.6	11
64	Solvent Effects on the Monomer/Hydrogenâ€Bonded Dimer Equilibrium in Carboxylic Acids: (+)â€(S)â€Ketopinic Acid as a Case Study. Chemistry - an Asian Journal, 2016, 11, 1798-1803.	3.3	11
65	Conformational landscape and hydrogen bonding in (S)-(â^')-perillyc acid: experimental VCD, IR, Raman, and theoretical DFT studies. Tetrahedron: Asymmetry, 2012, 23, 780-788.	1.8	10
66	Calculation of internal valence force constants for XY6(Oh) octahedral molecules. Journal of Molecular Structure, 1990, 220, 287-300.	3.6	9
67	Structural and vibrational study of isochroman. Chemical Physics, 2005, 313, 279-291.	1.9	9
68	An experimental and theoretical study of the molecular structure and vibrational spectra of iodotrimethylsilane (SiIMe3). Physical Chemistry Chemical Physics, 2006, 8, 477-485.	2.8	9
69	Effect of substituents and hydrogen bonding on barrier heights in dehydration reactions of carbon and silicon geminal diols. Physical Chemistry Chemical Physics, 2011, 13, 18507.	2.8	9
70	Studying the Effect of Temperature on the Formation of Hydrogen Bond Dimers: A FTIR and Computational Chemistry Lab for Undergraduate Students. Journal of Chemical Education, 2019, 96, 1760-1766.	2.3	9
71	Calculation of internal valence force constants for XY5 trigonal bipyramidal molecules. Journal of Molecular Structure, 1992, 265, 397-415.	3.6	8
72	Franckâ€“Condon factors and r-centroids for a number of band systems of the astrophysical molecule AlF. Astroparticle Physics, 2003, 20, 67-71.	4.3	8

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73	Dimethylsilanediol: Structure and vibrational spectra by IR and Raman spectroscopies and quantum chemical calculations. Vibrational Spectroscopy, 2012, 58, 79-86.	2.2	8
74	DFTâ€Aided Vibrational Circular Dichroism Spectroscopy Study of (â^')â€Sâ€cotinine. ChemPhysChem, 2015, 16, 1416-1427.	2.1	8
75	Pure vibrational force field for XYN branched molecules of high symmetry: Note in advance. Journal of Molecular Structure, 1990, 216, 297-300.	3.6	7
76	Mechanism of the Catalytic Activity of Nucleophiles in the Stepwise Hydrolysis and Condensation Reactions of Tetramethoxysilane. ChemPhysChem, 2009, 10, 940-945.	2.1	7
77	DFT predictions of vibrational spectra of titanium tetramethoxide oligomers and the structure of titanium tetraalkoxides in liquid and solid phases. Vibrational Spectroscopy, 2009, 51, 218-225.	2.2	7
78	Role of structures with penta- and hexacoordinate silicon in the nucleophile-catalyzed hydrolysis of tetramethoxysilane. Physical Chemistry Chemical Physics, 2009, 11, 841-847.	2.8	7
79	An assessment of DFT methods for predicting the thermochemistry of ion-molecule reactions of group 14 elements (Si, Ge, Sn). Journal of Molecular Modeling, 2013, 19, 5439-5444.	1.8	7
80	Vibrational spectra and electronic structure of germatranols (HO)4Ââ^'Ân Ge(OCH2CH2)nNR3Ââ^'Ân (RÂ=ÂH;) Tj ETQq0 0 0 rgBT /Overl	1.8	7
81	DFT study of the hydrolysis reaction in atranes and ocanes: the influence of transannular bonding. Journal of Molecular Modeling, 2016, 22, 3.	1.8	7
82	Structure and vibrational spectra of dimethylsilanediol and methylsilanetriol dimers. Chemical Physics Letters, 2005, 412, 359-364.	2.6	6
83	Anharmonic spectra of methanol and silanol: A comparative study. Journal of Molecular Spectroscopy, 2005, 233, 203-209.	1.2	6
84	Triethylsilanol:â€‰ Molecular Conformations and Role of the Hydrogen-Bonding Oligomerization in Its Vibrational Spectra. Journal of Physical Chemistry A, 2008, 112, 1545-1551.	2.5	6
85	Rotational strength sign and normal modes description: A theoretical and experimental comparative study in bicyclic terpenes. Chirality, 2010, 22, E123-9.	2.6	6
86	Characterization of H-bonding networks in chiral alcohols using Infrared, Raman and Vibrational Circular Dichroism spectroscopies, and density functional calculations: (S)-(â^')-perillyl alcohol. Tetrahedron: Asymmetry, 2012, 23, 515-525.	1.8	6
87	Quantum chemical study of silanediols as metal binding groups for metalloprotease inhibitors. Journal of Molecular Modeling, 2013, 19, 1819-1834.	1.8	6
88	Deducing the molecular properties of zwitterionic, protonated, deprotonated, and double-deprotonated forms of L-cysteine from vibrational spectroscopy (IR, Raman, VCD) and quantum chemical calculations. Journal of Molecular Modeling, 2014, 20, 2229.	1.8	6
89	Understanding the Aldoâ€Enediolate Tautomerism of Glycolaldehyde in Basic Aqueous Solutions. ChemPhysChem, 2015, 16, 2226-2236.	2.1	6
90	Conformational Flexibility of Limonene Oxide Studied By Microwave Spectroscopy. ChemPhysChem, 2017, 18, 268-268.	2.1	6

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91	A general quadratic force field for the out-of-plane vibrations of the s-tetrazine molecule. Spectrochimica Acta Part A: Molecular Spectroscopy, 1987, 43, 873-878.	0.1	5
92	A topological geometric method for the obtention of symmetry-adapted functions for point groups I. General theory. Computers and Mathematics With Applications, 1993, 26, 79-85.	2.7	5
93	Calculation of internal valence force constants for XY3Z (C3v) molecules. Journal of Molecular Structure, 1997, 407, 101-116.	3.6	5
94	A reinvestigation of the Î½7 and Î½10 modes of pyridazine on the basis of the inelastic neutron scattering spectrum analysis. Chemical Physics Letters, 2002, 361, 483-491.	2.6	5
95	The concept of canonical molecular force field. Journal of Molecular Structure, 2004, 705, 141-145.	3.6	5
96	Theoretical, ab initio and DFT, study of the structure and vibrational analysis of Raman, IR and INS spectra of (CH3)3SiNCO. Chemical Physics, 2006, 330, 26-42.	1.9	5
97	Conformations, Structures, and Vibrational Spectra of Triethylchloro- and Triethylbromosilane Using Theoretical Methods, Gas Phase Electron Diffraction, and IR and Raman Spectroscopy. Journal of Physical Chemistry A, 2007, 111, 2870-2878.	2.5	5
98	Conformational properties of chiral tobacco alkaloids by DFT calculations and vibrational circular dichroism: (â^')-S-anabasine. Journal of Molecular Graphics and Modelling, 2015, 60, 169-179.	2.4	5
99	A Mechanism-Based Sphingosine-1-phosphate Lyase Inhibitor. Journal of Organic Chemistry, 2020, 85, 419-429.	3.2	5
100	Franck-Condon factors and r-centroids for certain band systems of SiD, SiF and SiN molecules of astrophysical interest. Astronomy and Astrophysics, 1998, 129, 157-159.	2.1	5
101	A topological geometric method for the obtention of symmetry-adapted functions for point groups II. The icosahedral group. Computers and Mathematics With Applications, 1993, 26, 67-77.	2.7	4
102	Ab initio structural analysis of furylimidazoles. Computational and Theoretical Chemistry, 1997, 393, 97-110.	1.5	4
103	A set of force constants common for SiH3â€“X molecules. Journal of Molecular Structure, 1999, 482-483, 601-607.	3.6	4
104	Raman and IR spectra of the unstable ionic species potassium trimethylsilanolate: The role of the counterion in its theoretical interpretation. Journal of Raman Spectroscopy, 2008, 39, 460-467.	2.5	4
105	Conformational landscape of small organosilicon compounds from the combined use of gas electron diffraction, IR and Raman spectroscopies and quantum chemical calculations: diethyldichlorosilane. Journal of Raman Spectroscopy, 2010, 41, 1323-1330.	2.5	4
106	Molecular structure and vibrational spectra analysis of diethylsilanediol by IR and Raman spectroscopies and DFT calculations. Journal of Sol-Gel Science and Technology, 2012, 64, 54-66.	2.4	4
107	Interaction models of the Si(OH)2 functionality with Zn2+ cation in simplified biological environments: a DFT study. Structural Chemistry, 2014, 25, 127-138.	2.0	4
108	Synthesis and structural study of precursors of novel methylsilanediols by IR and Raman spectroscopies, single-crystal X-ray diffraction and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 828-834.	3.9	4

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109	Structural behavior of neutral, protonated, and deprotonated l-valine in aqueous solutions: a combined study using chirality sensitive (VCD) and non sensitive (IR and Raman) vibrational spectroscopies and quantum chemical calculations. Tetrahedron: Asymmetry, 2015, 26, 1314-1327.	1.8	4
110	Hyperconjugative and Electrostatic Interactions as Anomeric Triggers in Archetypical 1,4â€Đioxane Derivatives. ChemPhysChem, 2016, 17, 530-540.	2.1	4
111	The synergy of different solid-state techniques to elucidate the supramolecular assembly of two 1H-benzotriazole polymorphs. Physical Chemistry Chemical Physics, 2019, 21, 19879-19889.	2.8	4
112	A general quadratic force field for the pyridazine molecule: out-of-plane B1 normal modes. Journal of Molecular Structure, 1986, 142, 33-36.	3.6	3
113	A general quadratic force field for the s-trifluorotriazine molecule. Journal of Molecular Structure, 1986, 142, 37-40.	3.6	3
114	Icosahedral Matrix Representations as a Function of Eulerian Angles. Journal of Chemical Education, 1989, 66, 706.	2.3	3
115	Synthesis and structural study of ethylmethylsilanediol by quantum chemical calculations and IR and Raman spectroscopies. Journal of Sol-Gel Science and Technology, 2012, 61, 258-267.	2.4	3
116	Study of the chelating properties of Ge(OH)2 functionality as metal binding group for Zn2+ cation in simplified protease-like environments: a DFT analysis. Journal of Molecular Modeling, 2014, 20, 2430.	1.8	3
117	Validation of the Existence of Tetrameric Species of Potassium Trimethylsilanolate in the Gas Phase with a Theoretical Cluster Model:Â Role of the Counterion as Charge Localizer in the Structure. Journal of Physical Chemistry A, 2007, 111, 2629-2633.	2.5	2
118	Anomeric effect in pyranose-ring derivatives containing carbon, silicon, and germanium as anomeric centers: an ab initio systematic study. Structural Chemistry, 2019, 30, 2245-2255.	2.0	2
119	The icosahedral potential and its applications to the study of the anharmonic effects in the overtone levels of the degenerate vibrations of molecules with Ih symmetry. Monatshefte FÃ¼r Chemie, 1986, 117, 985-1001.	1.8	1
120	A revised application of the effective nuclear charge model to the prediction of force constants in trigonal-bipyramid XY5 molecules. Spectrochimica Acta Part A: Molecular Spectroscopy, 1987, 43, 703-708.	0.1	1
121	A study of series of force constants in the B3u and B2g symmetry species of s-tetrazine, using the display method. Spectrochimica Acta Part A: Molecular Spectroscopy, 1987, 43, 1257-1260.	0.1	1
122	A general quadratic force field for the diazirine molecule. Spectrochimica Acta Part A: Molecular Spectroscopy, 1987, 43, 447-449.	0.1	1
123	A topological geometric method for the obtention of symmetry-adapted functions for point groups IV. The dihedral groups. Computers and Mathematics With Applications, 1995, 29, 41-44.	2.7	1
124	Transition probabilities and dissociation energy of astrophysical molecule CoH. Astrophysics and Space Science, 2002, 280, 319-324.	1.4	1
125	Stabilizing factors of the molecular structure in silicon-based peptidomimetics in gas-phase and water solution. Assessment of the correlation between different descriptors of hydrogen bond strength. Journal of Molecular Modeling, 2013, 19, 4293-4304.	1.8	1
126	Quartic canonical force field in curvilinear internal coordinates for XY3 (D 3h) molecules. The case of the BH3 molecule. Journal of Molecular Modeling, 2014, 20, 2222.	1.8	0