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 Mechanism-Based Sphingosine-1-phosphate Lyase Inhibitor. Journal of Organic Chemistry, 2020, 85, 419-429.	3.2	5
2	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
3	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
4	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
5	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
6	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
7	Conformational Flexibility of Limonene Oxide Studied By Microwave Spectroscopy. ChemPhysChem, 2017, 18, 268-268.	2.1	6
8	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
9	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
10	Conformational Flexibility of Limonene Oxide Studied By Microwave Spectroscopy. ChemPhysChem, 2017, 18, 274-280.	2.1	15
11	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
12	Hyperconjugative and Electrostatic Interactions as Anomeric Triggers in Archetypical 1,4â€Dioxane Derivatives. ChemPhysChem, 2016, 17, 530-540.	2.1	4
13	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
14	Understanding the Aldoâ€Enediolate Tautomerism of Glycolaldehyde in Basic Aqueous Solutions. ChemPhysChem, 2015, 16, 2226-2236.	2.1	6
15	DFTâ€Aided Vibrational Circular Dichroism Spectroscopy Study of (â^')â€Sâ€cotinine. ChemPhysChem, 2015, 16, 1416-1427.	2.1	8
16	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
17	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
18	Vibrational Circular Dichroism and Theoretical Study of the Conformational Equilibrium in (â^')â€Sâ€Nicotine. ChemPhysChem, 2015, 16, 342-352.	2.1	12

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19	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
20	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
21	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
22	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
23	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
24	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
25	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
26	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
27	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
28	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
29	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
30	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
31	Quantum chemical study of silanediols as metal binding groups for metalloprotease inhibitors. Journal of Molecular Modeling, 2013, 19, 1819-1834.	1.8	6
32	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
33	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
34	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
35	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
36	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

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37	Selfâ€Assembly Structures of 1 H â€indazoles in the Solution and Solid Phases: A Vibrational (IR, FIR,) Tj ETQq1 1 0.784314 rgBT /Ove	2.1	14
38	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
39	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
40	Conformational landscape and hydrogen bonding in (S)-(âˆ’)-perillyc acid: experimental VCD, IR, Raman, and theoretical DFT studies. Tetrahedron: Asymmetry, 2012, 23, 780-788.	1.8	10
41	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
42	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
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	Conformational landscape of a chiral crown ether: a vibrational circular dichroism spectroscopy and computational study. Tetrahedron: Asymmetry, 2012, 23, 294-299.	1.8	11
45	Characterization of H-bonding networks in chiral alcohols using Infrared, Raman and Vibrational Circular Dichroism spectroscopies, and density functional calculations: (S)-(âˆ’)-perillyl alcohol. Tetrahedron: Asymmetry, 2012, 23, 515-525.	1.8	6
46	Dimethylsilanediol: Structure and vibrational spectra by IR and Raman spectroscopies and quantum chemical calculations. Vibrational Spectroscopy, 2012, 58, 79-86.	2.2	8
47	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
48	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
49	Chiral terpenes in different phases: R-(âˆ’)-camphorquinone studied by IRâ€“Ramanâ€“VCD spectroscopies and theoretical calculations. Structural Chemistry, 2011, 22, 67-76.	2.0	12
50	Structural and vibrational analyses of 2â€(2â€benzofuranyl)â€2â€imidazoline. Journal of Raman Spectroscopy, 2011, 42, 108-116.	2.5	33
51	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
52	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
53	Rotational strength sign and normal modes description: A theoretical and experimental comparative study in bicyclic terpenes. Chirality, 2010, 22, E123-9.	2.6	6
54	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

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55	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
56	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
57	Mechanism of the Catalytic Activity of Nucleophiles in the Stepwise Hydrolysis and Condensation Reactions of Tetramethoxysilane. ChemPhysChem, 2009, 10, 940-945.	2.1	7
58	Synthesis and vibrational analysis of Nâ€(2â€²â€Furyl)â€Imidazole. Journal of Raman Spectroscopy, 2009, 40, 1004-1010.	2.5	40
59	Structural and vibrational study of 4-(2â€²-furyl)-1-methylimidazole. Journal of Molecular Structure, 2009, 924-926, 322-331.	3.6	23
60	Structural and vibrational study of 2â€(2â€²â€•furyl)â€4,5â€‡Hâ€dihydroimidazole. Journal of Physical Organic Chemistry, 2009, 22, 1166-1177.	1.9	25
61	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
62	Conformational study of (R)-(+)-limonene in the liquid phase using vibrational spectroscopy (IR,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 4	1.8	47
63	Conformational landscape in chiral terpenes from vibrational spectroscopy and quantum chemical calculations: S-(+)-carvone. Vibrational Spectroscopy, 2009, 51, 318-325.	2.2	31
64	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
65	Conformational preference of a chiral terpene: vibrational circular dichroism (VCD), infrared and Raman study of S-(âˆ’)-limonene oxide. Physical Chemistry Chemical Physics, 2009, 11, 2459.	2.8	21
66	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
67	Structural and vibrational study of 2â€(2â€²â€furyl)â€‡Hâ€imidazole. Journal of Physical Organic Chemistry, 2008, 21, 1086-1097.	1.9	34
68	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
69	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
70	Conformational Flexibility in Terpenes: Vibrational Circular Dichroism (VCD), Infrared and Raman Study of S-(âˆ’)-Perillaldehyde. Journal of Physical Chemistry A, 2008, 112, 7887-7893.	2.5	38
71	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
72	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

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73	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
74	Photoinduced Chiral Nematic Organization in an Achiral Glassy Nematic Azopolymer. Advanced Functional Materials, 2007, 17, 3486-3492.	14.9	82
75	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
76	Structure and vibrational spectra of vinyl ether conformers. The comparison of B3LYP and MP2 predictions. Chemical Physics, 2007, 333, 148-156.	1.9	11
77	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
78	Vibrational spectra and structure of methoxysilanes and products of their hydrolysis. Vibrational Spectroscopy, 2006, 40, 1-9.	2.2	19
79	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
80	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
81	Vibrational spectrum of chlorotrimethylsilane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 62, 293-301.	3.9	12
82	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
83	Vibrational spectrum of methoxytrimethylsilane. Journal of Molecular Structure, 2005, 744-747, 331-338.	3.6	13
84	Structural and vibrational study of isochroman. Chemical Physics, 2005, 313, 279-291.	1.9	9
85	Structure and vibrational spectra of dimethylsilanediol and methylsilanetriol dimers. Chemical Physics Letters, 2005, 412, 359-364.	2.6	6
86	Anharmonic spectra of methanol and silanol: A comparative study. Journal of Molecular Spectroscopy, 2005, 233, 203-209.	1.2	6
87	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
88	Intramolecular hydrogen bonding in silanediols. Computational and Theoretical Chemistry, 2004, 678, 249-256.	1.5	16
89	Vibrational spectra of trimethylsilanol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2004, 60, 1169-1178.	3.9	26
90	The concept of canonical molecular force field. Journal of Molecular Structure, 2004, 705, 141-145.	3.6	5

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91	Hydrogen bonding and structure of silanediol dimers and tetramers. Chemical Physics Letters, 2004, 384, 326-331.	2.6	16
92	Intermolecular Charge Transfer and Hydrogen Bonding in Solid Furan. Journal of the American Chemical Society, 2004, 126, 15087-15095.	13.7	54
93	Condensation reactions in silanolâ€“water clusters. Chemical Physics Letters, 2003, 368, 616-624.	2.6	13
94	A new insight into the vibrational analysis of pyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 2815-2839.	3.9	121
95	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
96	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
97	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
98	Transition probabilities and dissociation energy of astrophysical molecule CoH. Astrophysics and Space Science, 2002, 280, 319-324.	1.4	1
99	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
100	Measurement and ab initio modeling of the inelastic neutron scattering of solid melamine. Chemical Physics, 2001, 266, 1-17.	1.9	50
101	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
102	Vibrational analysis of the inelastic neutron scattering spectrum of pyridine. Chemical Physics, 2000, 261, 239-247.	1.9	13
103	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
104	A set of force constants common for SiH3â€“X molecules. Journal of Molecular Structure, 1999, 482-483, 601-607.	3.6	4
105	Unambiguous formalism of molecular vibrations: Use of redundant coordinates and canonical matrices. Journal of Chemical Physics, 1999, 110, 3302-3308.	3.0	25
106	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
107	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
108	Ab initio structural analysis of furylimidazoles. Computational and Theoretical Chemistry, 1997, 393, 97-110.	1.5	4

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109	Calculation of internal valence force constants for XY3Z (C3v) molecules. Journal of Molecular Structure, 1997, 407, 101-116.	3.6	5
110	Vibrational analysis of the inelastic neutron scattering spectrum of s-triazine and trichloro-s-triazine. Chemical Physics, 1995, 200, 395-403.	1.9	25
111	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
112	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
113	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
114	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
115	Calculation of internal valence force constants for XY5 trigonal bipyramidal molecules. Journal of Molecular Structure, 1992, 265, 397-415.	3.6	8
116	Calculation of internal valence force constants for XY4 (Td) tetrahedral molecules. Journal of Molecular Structure, 1992, 271, 237-249.	3.6	11
117	Calculation of internal valence force constants for XY6(Oh) octahedral molecules. Journal of Molecular Structure, 1990, 220, 287-300.	3.6	9
118	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
119	Icosahedral Matrix Representations as a Function of Eulerian Angles. Journal of Chemical Education, 1989, 66, 706.	2.3	3
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 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
124	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
125	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
126	A general quadratic force field for the s-trifluorotriazine molecule. Journal of Molecular Structure, 1986, 142, 37-40.	3.6	3