Mauricio A Palafox

List of Publications by Year
in descending order

125	2,951	236833	182361
papers	citations	25 h-index	51 g-index

131	131	131	2275
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	How proton transfer affects the helical parameters in DNA:DNA microhelices. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13759-13777.	2.0	2
2	Studies on the molecular structure of pterocaronol: A new biologically relevant nor-triterpenoid from Peltophorum pterocarpum (Fabaceae). Journal of Molecular Structure, 2022, 1254, 132390.	1.8	0
3	New magnetic-fluorescent bifuntional (Y0.9Ln0.1VO4/Fe3O4)@SiO2 and [(Y0.9Ln0.1VO4@SiO2)/Fe3O4@SiO2] materials. Ceramics International, 2022, 48, 22006-22017.	2.3	4
4	Degradation of Human Serum Albumin by Infrared Free Electron Laser Enhanced by Inclusion of a Salen-Type Schiff Base Zn (II) Complex. International Journal of Molecular Sciences, 2020, 21, 874.	1.8	11
5	Developments in the Application of 1,2,3-Triazoles in Cancer Treatment. Recent Patents on Anti-Cancer Drug Discovery, 2020, 15, 92-112.	0.8	40
6	Structural transitions and bilayer formation of CTAB aggregates. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2019, 580, 123730.	2.3	13
7	Investigation by DFT Methods of the Damage of Human Serum Albumin Including Amino Acid Derivative Schiff Base Zn(II) Complexes by IR-FEL Irradiation. International Journal of Molecular Sciences, 2019, 20, 2846.	1.8	11
8	Effect of the sulfur atom on S2 and S4 positions of the uracil ring in different DNA:RNA hybrid microhelixes with three nucleotide base pairs. Biopolymers, 2019, 110, e23247.	1.2	9
9	FT-IR spectra of the anti-HIV nucleoside analogue d4T (Stavudine). Solid state simulation by DFT methods and scaling by different procedures. Journal of Molecular Structure, 2018, 1157, 587-601.	1.8	5
10	Effect of the sulphur atom on geometry and spectra of the biomolecule 2-thiouracil and in the WC base pair 2-thiouridine-adenosine. Influence of water in the first hydration shell. Journal of Biomolecular Structure and Dynamics, 2018, 36, 1225-1254.	2.0	3
11	FT-IR and FT-Raman spectra of 5-chlorocytosine: Solid state simulation and tautomerism. Effect of the chlorine substitution in the Watson-Crick base pair 5-chlorodeoxycytidine-deoxyguanosine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 188, 418-435.	2.0	6
12	Femtosecond laser reshaping yields gold nanorods with ultranarrow surface plasmon resonances. Science, 2017, 358, 640-644.	6.0	233
13	Density Functional Computations on 6-Aminouracil: Effect of Amino Group in the 6th Position on the Watsonâ€“Crick Base Pair Uridineâ€“Adenosine. Australian Journal of Chemistry, 2016, 69, 881.	0.5	2
14	Simulation of the solid state and the first and second hydration shell of the xanthine oxidase inhibitor allopurinol: Structures obtained using DFT and MP2 methods. Journal of Molecular Structure, 2016, 1111, 166-179.	1.8	2
15	6-Aminouracil: Geometries and spectra in the isolated state and in the solid state simulation. A comparison with 5-aminouracil. Journal of Molecular Structure, 2016, 1108, 482-495.	1.8	3
16	A DFT analysis of the molecular structure, vibrational spectra and other molecular properties of 5-nitrouracil and comparison with uracil. Journal of Molecular Structure, 2016, 1106, 300-315.	1.8	9
17	Theoretical Interpretation of Polarized Light-Induced Supramolecular Orientation on the Basis of Normal Mode Analysis of Azobenzene as Hybrid Materials in PMMA with Chiral Schiff Base Ni(II), Cu(II), and Zn(II) Complexes. Journal of Applied Solution Chemistry and Modeling, 2016, 5, 30-47.	0.4	11
18	Conformational analysis of the anti-HIV Nikavir prodrug: comparisons with AZT and Thymidine, and establishment of structureâ€“activity relationships/tendencies in other 6â€²-derivatives. Journal of Biomolecular Structure and Dynamics, 2015, 33, 723-748.	2.0	31

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19	FT-IR and FT-Raman spectra, MEP and HOMOâ€“LUMO of 2,5-dichlorobenzonitrile: DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 464-472.	2.0	29
20	Research Strategies Developed for the Treatment of Alzheimerâ€™s Disease. Reversible and Pseudo-Irreversible Inhibitors of Acetylcholinesterase: Structure-Activity Relationships and Drug Design. , 2014, , 426-477.		4
21	Structure and conformational analysis of the anti-HIV reverse transcriptase inhibitor AZT using MP2 and DFT methods. Differences with the natural nucleoside thymidine. Simulation of the 1st phosphorylation step with ATP. Physical Chemistry Chemical Physics, 2014, 16, 24763-24783.	1.3	8
22	FT-IR and FT-Raman spectra of 5-fluoroorotic acid with solid state simulation by DFT methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 132, 430-445.	2.0	6
23	FT-IR and FT-Raman spectra of 6-chlorouracil: Molecular structure, tautomerism and solid state simulation. A comparison between 5-chlorouracil and 6-chlorouracil. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 130, 653-668.	2.0	17
24	FT-IR, FT-Raman spectra and other molecular properties of 2,4- dichlorobenzonitrile: A interpretation by a DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 123, 89-97.	2.0	7
25	Molecular structure differences between the antiviral Nucleoside Analogue 5-iodo-2â€²-deoxyuridine and the natural nucleoside 2â€²-deoxythymidine using MP2 and DFT methods: conformational analysis, crystal simulations, DNA pairs and possible behaviour. Journal of Biomolecular Structure and Dynamics, 2014, 32, 831-851.	2.0	37
26	Anticancer drug IUdR and other 5-halogen derivatives of 2â€²-deoxyuridine: conformers, hydrates, and structureâ€“activity relationships. Structural Chemistry, 2014, 25, 53-69.	1.0	10
27	Conformational Analysis, Molecular Structure and Solid State Simulation of the Antiviral Drug Acyclovir (Zovirax) Using Density Functional Theory Methods. Pharmaceuticals, 2014, 7, 695-722.	1.7	15
28	Research Strategies Developed for the Treatment of Alzheimerâ€™s Disease. Reversible and Pseudo-Irreversible Inhibitors of Acetylcholinesterase: Structure-Activity Relationships and Drug Design. , 2014, , 426-477.		1
29	Structureâ€“activity relationships of the antiviral D4T and seven 4â€²-substituted derivatives using MP2 and DFT methods. Structural Chemistry, 2013, 24, 967-980.	1.0	6
30	The biomolecule of 5-bromocytosine: FT-IR and FT-Raman spectra and DFT calculations. Identification of the tautomers in the isolated state and simulation the spectra in the solid state. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 111, 104-122.	2.0	13
31	Effect of the microhydration on the tautomerism in the anticarcinogenic drug 5-fluorouracil and relationships with other 5-haloderivatives. Journal of Molecular Structure, 2013, 1054-1055, 32-45.	1.8	18
32	Simulation of a tetramer form of 5-chlorouracil: The vibrational spectra and molecular structure in the isolated and in the solid state by using DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 110, 404-418.	2.0	12
33	Molecular structure of the nucleoside analogue inosine using DFT methods: Conformational analysis, crystal simulations and possible behaviour. Journal of Molecular Structure, 2013, 1047, 358-371.	1.8	12
34	FT-IR, FT-Raman spectra and other molecular properties of 3,5-dichlorobenzonitrile: A DFT study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 116, 509-517.	2.0	10
35	Vibrational spectral investigations and density functional theory study of 4-Formylbenzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 114, 502-508.	2.0	7
36	2-Amino-3,5-dichlorobenzonitrile: DFT calculations in the monomer and dimer forms, FT-IR and FT-Raman spectra, molecular geometry, atomic charges and thermodynamical parameters. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 110, 458-470.	2.0	6

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37	Solid state simulation of tetramer form of 5-aminoorotic acid: The vibrational spectra and molecular structure study by using MP2 and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 97, 948-962.	2.0	11
38	Structure of the antiviral stavudine using quantum chemical methods: Complete conformational space analysis, 3D potential energy surfaces and solid state simulations. Journal of Molecular Structure, 2012, 1028, 181-195.	1.8	13
39	Tautomerism in 5-Bromouracil: Relationships with Other 5-Haloderivatives and Effect of the Microhydration. Spectroscopy Letters, 2011, 44, 300-306.	0.5	18
40	Structure and conformational analysis of the anti-HIV AZT 5â€²-aminocarbonylphosphonate prodrug using DFT methods. Chemical Physics, 2011, 387, 11-24.	0.9	14
41	DFT calculation of four new potential agents muscarinic of bispyridinium type: structure, synthesis, biological activity, hydration, and relations with the potents W84 and DUO-3O. Journal of Computer-Aided Molecular Design, 2011, 25, 145-161.	1.3	19
42	Density functional theory calculations and vibrational spectral analysis of 3,5-(dinitrobenzoic acid). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 1437-1444.	2.0	59
43	Vibrational spectra, tautomerism and thermodynamics of anticarcinogenic drug: 5-Fluorouracil. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 79, 970-977.	2.0	44
44	Vibrational spectra, normal coordinate analysis and thermodynamics of 2, 5-difluorobenzonitrile. Indian Journal of Physics, 2010, 84, 151-165.	0.9	11
45	Relationships observed in the structure and spectra of uracil and its 5-substituted derivatives. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2010, 75, 1261-1269.	2.0	38
46	FT-IR and FT-Raman spectra, ab initio and density functional computations of the vibrational spectra, molecular geometry, atomic charges and some molecular properties of the biomolecule 5-iodouracil. Computational and Theoretical Chemistry, 2010, 940, 29-44.	1.5	21
47	Simulation of a tetramer form of 5-iodouracil: The vibrational spectra and molecular structure in the isolated and in the solid state by using DFT calculations. Vibrational Spectroscopy, 2010, 52, 108-121.	1.2	15
48	Raman and Infrared Spectra of Hydrated 2,4-Dithiouracil Molecule. , 2010, , .		2
49	FT-IR and FT-Raman spectra of complex of La(III) with 6-aminouracil. , 2010, , .		0
50	Hydrogen Bond Analysis of L-Ascorbic Acid: Ab Initio Study. , 2010, , .		0
51	Raman And Infrared Spectra Of Hydrated 5-Nitrouracil Molecule. , 2010, , .		1
52	FT-IR and FT-Raman Spectra of 2, 6-Difluorobenzonitrile. , 2010, , .		0
53	Quantum Chemical Scaling and Its Importance: The Infrared and Raman Spectra of 5-Bromouracil. Spectroscopy Letters, 2010, 43, 51-59.	0.5	20
54	Hydration Analysis of Antiviral Agent AZT by Means of DFT and MP2 Calculations. Journal of Physical Chemistry B, 2010, 114, 15199-15211.	1.2	19

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55	Tautomerism of the natural thymidine nucleoside and the antiviral analogue D4T. Structure and influence of an aqueous environment using MP2 and DFT methods. Physical Chemistry Chemical Physics, 2010, 12, 881-893.	1.3	27
56	Simulation of the First Hydration Shell of Nucleosides D4T and Thymidine: Structures Obtained Using MP2 and DFT Methods. Journal of Physical Chemistry B, 2009, 113, 2458-2476.	1.2	38
57	On the Connection between the Complexation and Aggregation Thermodynamics of Oxyethylene Nonionic Surfactants. Journal of Physical Chemistry B, 2008, 112, 15691-15700.	1.2	12
58	FTIR and FTâ€Raman spectra and density functional computations of the vibrational spectra, molecular geometry and atomic charges of the biomolecule: 5â€bromouracil. Journal of Raman Spectroscopy, 2007, 38, 1227-1241.	1.2	79
59	Studying the transfer process of a gemini surfactant from water to Î²-cyclodextrin at a molecular level. Chemical Physics Letters, 2007, 446, 92-97.	1.2	13
60	Geometrical parameters, vibrational wavenumbers, and relationships established with six difluorobenzonitriles. International Journal of Quantum Chemistry, 2007, 107, 1099-1114.	1.0	16
61	FT-IR, FT-Raman spectra, density functional computations of the vibrational spectra and molecular geometry of biomolecule 5-aminouracil. Chemical Physics, 2007, 340, 17-31.	0.9	98
62	IR and Raman spectra, density functional computations of vibrational spectrum, molecular geometry, atomic charges, and some molecular properties of 3-aminobenzonitrile molecule. International Journal of Quantum Chemistry, 2006, 106, 1885-1901.	1.0	11
63	Unexpected binding mode of gemini surfactants and Î³-cyclodextrin: DOSY as a tool for the study of complexation. Chemical Physics Letters, 2006, 432, 486-490.	1.2	19
64	4-Aminobenzonitrile:ab initio calculations, FTIR and Raman spectra. Journal of Raman Spectroscopy, 2006, 37, 85-99.	1.2	22
65	Scaling factors for the prediction of vibrational spectra. II. The aniline molecule and several derivatives. International Journal of Quantum Chemistry, 2005, 103, 394-421.	1.0	157
66	Benzonitriles: Survey of Their Importance and Scaling of Their Vibrational Frequencies. ChemInform, 2003, 34, no.	0.1	0
67	Vibrational frequencies and structure of 2-thiouracil by Hartreeâ€"Fock, post-Hartreeâ€"Fock and density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 2473-2486.	2.0	56
68	Benzonitriles: Survey of their importance and scaling of their vibrational frequencies. International Journal of Quantum Chemistry, 2003, 94, 189-204.	1.0	51
69	Quantum chemical predictions of the vibrational spectra of polyatomic molecules.. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 411-440.	2.0	168
70	3,5-Difluorobenzonitrile: ab initio calculations, FTIR and Raman spectra. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2002, 58, 1987-2004.	2.0	170
71	The hydration effect on the uracil frequencies: an experimental and quantum chemical study. Computational and Theoretical Chemistry, 2002, 585, 69-92.	1.5	66
72	Accurate scaling of the vibrational spectra of aniline and several derivatives. Computational and Theoretical Chemistry, 2002, 593, 101-131.	1.5	100

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73	Theoretical quantum chemical study of benzoic acid: Geometrical parameters and vibrational wavenumbers. International Journal of Quantum Chemistry, 2002, 89, 1-24.	1.0	37
74	Quantum chemical study of several monocyclic complex Î²-lactam C-3, C-4, and N-derivatives, and Î²-ring model molecules. International Journal of Quantum Chemistry, 2002, 89, 25-47.	1.0	6
75	Study of phenothiazine andN-methyl phenothiazine by infrared, raman,1H-, and13C-NMR spectroscopies. International Journal of Quantum Chemistry, 2002, 89, 147-171.	1.0	27
76	Laser Raman and IR spectra and force fields for 2,4-dichlorobenzonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 209-216.	2.0	14
77	Ab initio calculations, FTIR and Raman spectra of 2,3-difluorobenzonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2001, 57, 2373-2389.	2.0	19
78	FTIR study of five complex Î²-lactam molecules. Biopolymers, 2001, 62, 278-294.	1.2	6
79	Scaling factors for the prediction of vibrational spectra. I. Benzene molecule. International Journal of Quantum Chemistry, 2000, 77, 661-684.	1.0	405
80	Fourier transform Raman spectrum andab initio and density functional computations of the vibrational spectrum, molecular geometry, atomic charges and some molecular properties of the anticarcinogenic drug 5-fluorouracil. Journal of Raman Spectroscopy, 2000, 31, 595-603.	1.2	50
81	FTIR and FT-Raman spectra of 5-methyluracil (thymine). Journal of Raman Spectroscopy, 2000, 31, 1005-1012.	1.2	48
82	Ab initio study of geometrical structures of SiH3â€“XH silanes. Computational and Theoretical Chemistry, 2000, 528, 269-285.	1.5	6
83	Scaling factors for the prediction of vibrational spectra. I. Benzene molecule. International Journal of Quantum Chemistry, 2000, 77, 661.	1.0	12
84	A reinvestigation of the molecular structure of dimethyl- N -nitramine by gas electron diffraction, ab initio calculations of the molecular geometry and the force field and vibrational spectra. Journal of Molecular Structure, 1999, 485-486, 153-161.	1.8	4
85	A comparative study of the scaled vibrational frequencies in the local anesthetics procaine, tetracaine and propoxycaine by means of semiempirical methods: AM1, PM3 and SAM1. Computational and Theoretical Chemistry, 1999, 459, 239-271.	1.5	19
86	Inter-relationships between the geometrical parameters of the amino group in several para -substituted anilines. Computational and Theoretical Chemistry, 1999, 493, 171-177.	1.5	22
87	Geometry and frequencies of the halothane molecule. Computational and Theoretical Chemistry, 1999, 493, 179-185.	1.5	8
88	Scaling Factors for the Prediction of the Frequencies of the Ring Modes in Benzene Derivatives. Journal of Physical Chemistry A, 1999, 103, 11366-11377.	1.1	36
89	Classical and Inverted Structures of SiXnH3-nLi and SiXnH3-nNa. Journal of Physical Chemistry A, 1999, 103, 8537-8542.	1.1	6
90	Infrared Study of Phenothiazine and N-Methyl Phenothiazine. , 1999, , 611-612.		0

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91	Synthesis and characterisation of complex of Cu(II) with 6-azauracil. , 1999, , 637-638.		0
92	Quantum Chemical Predictions of the NMR Spectrum of Phenothiazine and N-Methyl Phenothiazine. , 1999, , 433-434.		0
93	Vibrational study of Î±- and Î³-pyridone. , 1999, , 613-614.		0
94	Uracil molecule: the transferability of the scale factors for the prediction of the infrared spectra. , 1999, , 295-296.		0
95	Synthesis and characterisation of complex of Cu(II) with 5-carboxy-2-thiouracil. , 1999, , 625-626.		0
96	Vibrational study of 3-methyluracil. , 1999, , 293-294.		0
97	Structures and Spectral Characteristics of Silylborane, Silylaluminum Hydride, Silylphosphine, and Silyl Mercaptan. Spectroscopy Letters, 1997, 30, 379-402.	0.5	5
98	Raman Spectrum of Procaine Hydrochloride. Spectroscopy Letters, 1997, 30, 975-998.	0.5	10
99	Interpretation of the vibrational spectra of chloramide, H2NCl, on the basis of post-Hartree-Fock force field. Computational and Theoretical Chemistry, 1997, 417, 187-193.	1.5	2
100	A Spectroscopic Study of Several Î²-Lactams by FT-IR and Theoretical Methods. , 1997, , 533-534.		0
101	A Study of Para-Aminobenzoic Acid: Structure, Frequencies, Torsion and Inversion Barriers of the Amino Group. , 1997, , 535-536.		1
102	Frequencies and Structure of the 1,3-Deimethyluracil Devier. , 1997, , 215-216.		0
103	Characterization of the Î²-Lactam Ring Fundamental Vibrations by Ab Initio and FT-IR Methods. , 1995, , 79-80.		0
104	Infrared and Raman Study of the Local Anesthetic Procaine. Spectroscopy Letters, 1994, 27, 613-638.	0.5	13
105	Eclipsed and staggered conformations of (SIH3)2F+: An ab initio study. International Journal of Quantum Chemistry, 1994, 50, 69-90.	1.0	3
106	Dimer form of 1,3-dimethyluracil studied by theAM1 semiempirical method. International Journal of Quantum Chemistry, 1994, 51, 141-159.	1.0	3
107	Vibrational frequencies, conformations and geometry of procaine. Vibrational Spectroscopy, 1994, 6, 149-165.	1.2	9
108	Inverse bond length/bond angle relationships. Computational and Theoretical Chemistry, 1994, 304, 261-267.	1.5	4

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109	Spectroscopy of p-Methoxybenzoic Acid: An AM1 and ab Initio Study. Applied Spectroscopy, 1994, 48, 27-36.	1.2	20
110	Comparison Between the IR Spectra and the Structure of the Two Conformations of a Diazabicyclanol. Spectroscopy Letters, 1994, 27, 1165-1186.	0.5	3
111	Nonempirical quantum chemical calculation for nitramide, its chloro- and methyl-substituted derivatives. I. Structure of equilibrium forms. Journal of Structural Chemistry, 1993, 34, 2-8.	0.3	5
112	An AM1 study of structure and conformational isomerism in bicyclo[3.3.1]nonane and several 3,7-diaza derivatives. Computational and Theoretical Chemistry, 1993, 285, 33-46.	1.5	4
113	Theoretical prediction of the vibrational spectrum, geometry, and scaled quantum mechanical (SQM) force field of phenylsilane, C6H5SiH3. Computational and Theoretical Chemistry, 1993, 284, 23-35.	1.5	6
114	Structure and spectral characteristics of o-aminobenzoic acid by AM1. Vibrational Spectroscopy, 1993, 6, 95-105.	1.2	35
115	Infrared and Raman Study of Benzocaine Hydrochloride. Spectroscopy Letters, 1993, 26, 1395-1415.	0.5	2
116	Conformational study of several diazabicyclanols by the AM1 method. Computational and Theoretical Chemistry, 1992, 257, 259-278.	1.5	2
117	A comparative study of the procaineâ€"H+ structures. Interpretation of the procaine hydrochloride spectra by AM1. Computational and Theoretical Chemistry, 1992, 262, 7-20.	1.5	3
118	AM1 study of several diazabicyclanones. Computational and Theoretical Chemistry, 1992, 262, 21-37.	1.5	2
119	Structural and vibrational study of the 3,7-dimethyl-3,7- diazabicyclo [3.3.1] nonan-9-ol molecule by the AM1 method. Journal of Molecular Structure, 1991, 249, 313-325.	1.8	3
120	A comparative study of the vibrational frequencies and intensities in benzocaine by means of semiempirical methods: AM1, MINDO/3 and MNDO. Computational and Theoretical Chemistry, 1991, 236, 161-192.	1.5	33
121	Conformational changes by ring puckering and inversion in 1,3,2-dioxaphospholene. Computational and Theoretical Chemistry, 1991, 228, 315-322.	1.5	1
122	Raman spectra and vibrational analysis for benzocaine. Journal of Raman Spectroscopy, 1989, 20, 765-771.	1.2	13
123	Calculation of the transitions in the amine inversion vibration of some local anesthetics. Journal of Molecular Structure, 1988, 175, 81-84.	1.8	10
124	Infrared study of some solid local anesthetics. Spectrochimica Acta Part A: Molecular Spectroscopy, 1988, 44, 1465-1471.	0.1	10
125	Laser Raman spectroscopy of some local anesthetics. Journal of Molecular Structure, 1986, 143, 415-418.	1.8	2