Peter Klaeboe

List of Publications by Year
in descending order

123	1,317	430874 18	501196 28
papers	citations	h-index	g-index

124	124	124	698
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Spectra and structure of silicon-containing compounds. XXXVI?Raman and infrared spectra, conformational stability,ab initio calculations and vibrational assignment of ethyldibromosilane. Journal of Raman Spectroscopy, 2003, 34, 322-336.	2.5	96
2	Conformational studies by vibrational spectroscopy: a review of various methods. Vibrational Spectroscopy, 1995, 9, 3-17.	2.2	54
3	The vibrational spectra of maleimide and N-D maleimide. Journal of Molecular Structure, 1975, 27, 283-301.	3.6	48
4	Infrared emission spectra of alkali chloroaluminates and related melts. Inorganic Chemistry, 1984, 23, 706-715.	4.0	44
5	The vibrational spectra, molecular structure and conformations of organic azides. I. A survey. Journal of Molecular Structure, 1986, 141, 161-172.	3.6	43
6	The i.r., Raman and microwave spectra of 1-butene-3-yne (vinylacetylene) and 1-butene-3-yne-4d. Spectrochimica Acta Part A: Molecular Spectroscopy, 1980, 36, 975-987.	0.1	42
7	Infrared study of CO adsorbed on Co/Î³-Al2O3 based Fischerâ€“Tropsch catalysts; semi-empirical calculations as a tool for vibrational assignments. Physical Chemistry Chemical Physics, 2000, 2, 1835-1846.	2.8	38
8	The vibrational spectra, molecular structure and conformation of organic azides. Journal of Molecular Structure, 1986, 147, 203-215.	3.6	28
9	The virbrational spectra, molecular structure and conformations of organic azides. Journal of Molecular Structure, 1987, 160, 1-26.	3.6	28
10	The vibrational spectra, molecular structure and conformation of organic azides. Journal of Molecular Structure, 1986, 147, 217-229.	3.6	24
11	Spectroscopic studies of ethylene-propylene copolymers in the near- and mid-infrared regions. Vibrational Spectroscopy, 1992, 3, 23-33.	2.2	23
12	Far infrared spectra, conformational equilibria, vibrational assignments and ab initio calculations of 2-chloroethanol. Journal of Molecular Structure, 1996, 385, 7-21.	3.6	23
13	The conformation and vibrational spectra of trans-1,4-dihalocyclohexanes. Journal of Molecular Structure, 1980, 66, 31-43.	3.6	22
14	The vibrational and NMR spectra, conformations and ab initio calculations of aminomethylene, propanedinitrile and itsN-methyl derivatives. Structural Chemistry, 1996, 7, 17-36.	2.0	22
15	Vibrational spectra, conformations, quantum chemical calculations and spectral assignments of 1-chloro-1-silacyclohexane. Vibrational Spectroscopy, 2012, 61, 167-175.	2.2	21
16	Condensed Aromatics. Part VII. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 1980, 35, 1390-1394.	1.5	20
17	Infrared and Raman spectra, conformations, ab initio calculations and spectral assignments of 1-fluoro-1-silacyclohexane. Journal of Molecular Structure, 2012, 1015, 120-128.	3.6	19
18	Infrared and Raman spectra, conformations, quantum chemical calculations and spectral assignments of 1-methyl-1-silacyclohexane. Journal of Molecular Structure, 2013, 1034, 207-215.	3.6	19

#	Article	IF	Citations
19	The molecular structure, conformations and vibrational spectra of 2,2-di(chloromethyl)-1,3-dichloropropane and 2,2-di(bromomethyl)-1,3-dibromopropane. Journal of Molecular Structure, 1986, 140, 1-18.	3.6	18
20	Vibrational spectroscopic study of 2-fluorophenol and 2,3,5,6-tetrafluorohydroquinone. Chemical Physics, 2007, 335, 205-214.	1.9	18
21	Vibrational and high pressure conformational studies of 1,1,2-trichloroethane. Journal of Molecular Structure, 1976, 34, 33-45.	3.6	17
22	The vibrational spectra, molecular structure and conformation of organic azides. Computational and Theoretical Chemistry, 1989, 200, 443-462.	1.5	16
23	Vibrational spectra and conformations of chloro- and bromo-cyclobutane. Journal of Raman Spectroscopy, 1989, 20, 239-250.	2.5	16
24	The conformations of bromomethyl dimethyl silane and bromomethyl dimethyl silane-d1 as studied by vibrational spectroscopy and by ab initio calculations. Vibrational Spectroscopy, 1998, 17, 1-30.	2.2	16
25	Infrared and Raman spectra, DFT-calculations and spectral assignments of silacyclohexane. Journal of Molecular Structure, 2012, 1023, 189-196.	3.6	16
26	The IR matrix isolation spectra and conformation energies of eight haloacetylhalides (CH2X-COY; X, Y) Tj ETQq0 0 0 rgBT /Overlock 10 T	3.6	15
27	The vibrational spectra of N-Cl maleimide. Journal of Molecular Structure, 1975, 28, 269-278.	3.6	14
28	The vibrational spectra, molecular structure and conformation of organic azides. Journal of Molecular Structure, 1987, 160, 245-257.	3.6	13
29	The vibrational spectra including matrix isolation and conformations of 1-chloro-1-fluorocyclobutane and 1-chloro-1,2,2-trifluorocyclobutane. Journal of Molecular Structure, 1993, 300, 209-232.	3.6	13
30	The conformers of chloromethyl dimethyl fluorosilane studied by vibrational spectroscopy and ab initio methods. Journal of Molecular Structure, 1998, 445, 161-178.	3.6	13
31	The conformations, phase transitions and vibrational spectra of bicyclohexyl. Spectrochimica Acta Part A: Molecular Spectroscopy, 1986, 42, 1141-1154.	0.1	12
32	Far Infrared Spectra, Conformational Equilibrium, Barriers to Internal Rotation, Vibrational Assignment and ab initio Calculations of 2-Fluoroethanol. Zeitschrift Fur Physikalische Chemie, 1995, 191, 23-45.	2.8	12
33	Diffuse reflectance IR studies of bimetallic Fischer-Tropsch catalysts. Journal of Molecular Structure, 1995, 349, 325-328.	3.6	12
34	Study of the conformers of dichloromethylmethyldifluorosilane by vibrational spectroscopy andab initio methods. Journal of Raman Spectroscopy, 1998, 29, 627-643.	2.5	12
35	Spectra and structure of silicon containing compounds. XXXIX. Raman and infrared spectra, conformational stability, vibrational assignment and ab initio calculations of n -propyltrifluorosilane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2003, 59, 2151-2173.	3.9	12
36	Raman and infrared spectra, quantum chemical calculations, conformations and spectral assignments of 1-chloro-1-methyl-1-silacyclohexane. Journal of Molecular Structure, 2013, 1047, 282-291.	3.6	12

#	Article	IF	Citations
37	The conformation and vibrational spectra of 1,5-hexadiene-3-yne (divinylacetylene) and perchloro-1,5-hexadiene-3-yne (perchlorodivinylacetylene). Journal of Molecular Structure, 1981, 71, 71-89.	3.6	11
38	The vibrational spectra of 1-chloro-2,2-dimethylpropane. Spectrochimica Acta Part A: Molecular Spectroscopy, 1985, 41, 1315-1319.	0.1	11
39	The vibrational spectra, molecular structure and conformation of organic azides. Journal of Molecular Structure, 1988, 176, 107-122.	3.6	11
40	Vibrational spectroscopic studies, conformations andab initio calculations of 1,1,1-trifluoropropyltrifluorosilane. Journal of Raman Spectroscopy, 2003, 34, 711-724.	2.5	11
41	Infrared and Raman Spectra and Conformational Equilibrium of Chloromethyl Dimethyl Chlorosilane.. Acta Chemica Scandinavica, 1998, 52, 578-592.	0.7	11
42	IR Matrix isolation studies of the conformations of 1,3-dichloro-2,2-dimethylpropane and 2-(chloromethyl)-2-methyl-1,3-dichloropropane. Journal of Molecular Structure, 1990, 218, 67-72.	3.6	10
43	Vibrational spectra of seven halomethanes. Analyst, The, 1992, 117, 365-369.	3.5	10
44	Infrared and Raman spectroscopy applied to conformational equilibria; methods and recent results. Journal of Molecular Structure, 1997, 408-409, 81-89.	3.6	10
45	Vibrational spectra, conformational equilibrium and ab initio calculations of 1,2-diphenylethane. Journal of Molecular Structure, 2004, 695-696, 77-94.	3.6	10
46	Raman and far infrared spectra and conformation of 1,2-diiodotetrafluoroethane. Journal of Raman Spectroscopy, 1978, 7, 111-114.	2.5	9
47	Vibrational spectra of the charge transfer complexes between organic sulfides and iodine. Spectrochimica Acta Part A: Molecular Spectroscopy, 1984, 40, 351-359.	0.1	9
48	The conformers of chloromethylmethyldifluorosilane studied by vibrational spectroscopy andab initio methods. Journal of Raman Spectroscopy, 2000, 31, 897-907.	2.5	9
49	Conformational equilibria, Raman and infrared spectra andab initio calculations of dichloromethylmethyldichlorosilane. Journal of Raman Spectroscopy, 2001, 32, 303-318.	2.5	9
50	Vibrational spectroscopic studies, conformations andab initio calculations ofn-propyltrichlorosilane. Journal of Raman Spectroscopy, 2004, 35, 975-990.	2.5	9
51	The Conformational Equilibria and Vibrational Spectra, Including Infrared Matrix Isolation Spectra, of Chloroacetyl Chloride and Chloroacetyl Bromide.. Acta Chemica Scandinavica, 1991, 45, 877-886.	0.7	9
52	Conformational Properties of 2-Cyclopropylideneethanol as Studied by Microwave, Infrared and Raman Spectroscopy and by Ab Initio Computations.. Acta Chemica Scandinavica, 1998, 52, 1122-1136.	0.7	9
53	The conformational equilibria and the IR and Raman spectra of 2-(choromethyl)-2-methyl-1,3-dichloropropane. Journal of Raman Spectroscopy, 1986, 17, 437-446.	2.5	8
54	Vibrational spectra, phase transitions and conformers of 1,4-dichlorobut-2-yne. Journal of Raman Spectroscopy, 1987, 18, 461-471.	2.5	8

#	Article	IF	Citations
55	The vibrational spectra of hexafluorocyclobutene and 1,2-dichlorotetrafluorocyclobutene. Spectrochimica Acta Part A: Molecular Spectroscopy, 1987, 43, 983-989.	0.1	8
56	Recent advances in infrared matrix isolation spectroscopy. Invited lecture. Analyst, The, 1992, 117, 335.	3.5	8
57	Solid phases of bicyclohexyl studied with vibrational spectroscopy and calorimetry. Analyst, The, 1992, 117, 355.	3.5	8
58	Vibrational spectra including matrix isolation and conformations of 1,1,2-trichloro-2,3,3-trifluorocyclobutane. Journal of Molecular Structure, 1993, 295, 73-94.	3.6	8
59	Title is missing!. Structural Chemistry, 1999, 10, 1-15.	2.0	8
60	Infrared and Raman spectra, ab initio calculations and conformational equilibria of chloromethyl methyl dichlorosilane. Journal of Molecular Structure, 2001, 597, 137-155.	3.6	8
61	Infrared and Raman Spectra, conformations,ab initio calculations and spectral assignments of 1,3-disilabutane (SiH3CH2SiH2CH3). Journal of Raman Spectroscopy, 2007, 38, 1159-1173.	2.5	8
62	The infrared and Raman spectra, ab initio calculations and spectral assignments of cyclopropylmethyl dichlorosilane (c-C3H5)SiCl2CH3. Vibrational Spectroscopy, 2011, 56, 136-145.	2.2	8
63	The vibrational spectra of cis- and trans-1-chloro-1,3-butadiene. Spectrochimica Acta Part A: Molecular Spectroscopy, 1980, 36, 119-130.	0.1	7
64	The vibrational spectra and conformations of polyhalogenated cyclobutanes. Journal of Molecular Structure, 1990, 218, 51-58.	3.6	7
65	Conformational equilibrium in dimethyl vinyl fluorosilane studied by infrared and Raman spectroscopy. Journal of Molecular Structure, 2000, 554, 251-269.	3.6	7
66	Spectra and structure of silicon containing compounds. XXXI. Raman and infrared spectra, conformational stability, ab initio calculations, and vibrational assignment of ethyl bromosilane and ethyl bromosilane-Si-d2. Journal of Molecular Structure, 2002, 641, 125-146.	3.6	7
67	Vibrational spectroscopic studies, conformations and quantum chemical calculations of 3,3,3-trifluoropropyl- silane and 3,3,3-trifluoropropylsilane-d3. Journal of Raman Spectroscopy, 2006, 37, 29-51.	2.5	7
68	Vibrational spectra, ab initio calculations and vibrational assignments of 3-butyn-1-ol. Journal of Molecular Structure, 2008, 886, 90-102.	3.6	7
69	Infrared and Raman spectra, DFT-calculations and spectral assignments of 1,3,5-trisilacyclohexane. Journal of Molecular Structure, 2014, 1076, 419-425.	3.6	7
70	The vibrational spectra and force constant calculations of ethynylcyclohexane. Spectrochimica Acta Part A: Molecular Spectroscopy, 1985, 41, 43-52.	0.1	6
71	In situ investigation of solid state Ion exchange in zeolites using Fourier transform infrared spectroscopy. Analyst, The, 1992, 117, 351.	3.5	6
72	Vibrational and rotational spectra and ab initio calculations of thiocyanatoethene. Journal of Molecular Structure, 1995, 349, 37-40.	3.6	6

#	Article	IF	Citations
73	Conformational stability, vibrational spectra and ab initio calculations for chloromethyl methyl silane and chloromethyl methyl difluorosilane. Journal of Molecular Structure, 1999, 480-481, 147-151.	3.6	6
74	Vibrational spectroscopic studies, conformations and ab initio calculations of 3,3,3-trifluoropropyltrichlorosilane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 1335-1346.	3.9	6
75	Vibrational spectroscopic studies, conformations and ab initio calculations of 1,2â€bis(trifluorosilyl)ethane (SiF₃CH₂CH₂SiF₃). Journal of Raman Spectroscopy, 2009, 40, 2111-2122.	2.5	6
76	Untersuchung von Konformationsgleichgewichten und WasserstoffbrÃ¼ckenbindungen mit Hilfe der Hochdruckschwingungsspektroskopie. Zeitschrift FÃ¼r Chemie, 1981, 21, 381-387.	0.0	6
77	The Conformers of Bromomethyl Dimethyl Fluorosilane Studied by Vibrational Spectroscopy and ab Initio Methods.. Acta Chemica Scandinavica, 1998, 52, 1359-1372.	0.7	6
78	The vibrational spectra and conformation of six trans-1,4-dihalocyclohexanes(Cl, Br, I). Journal of Molecular Structure, 1980, 60, 121-126.	3.6	5
79	The vibrational spectrum of propyne-3d1. Spectrochimica Acta Part A: Molecular Spectroscopy, 1980, 36, 1017-1020.	0.1	5
80	The conformational equilibria and vibrational spectra, including infrared matrix-isolation spectra, of fluoroacetyl chloride and fluoroacetyl bromide. Journal of Molecular Structure, 1992, 273, 27-48.	3.6	5
81	Vibrational spectra and conformations of 2,2-di(fluoromethyl)-1,3-difluoropropane and assignments based upon ab initio force fields. Journal of Raman Spectroscopy, 1993, 24, 303-315.	2.5	5
82	Infrared and Raman spectra, ab initio calculations and conformational studies of ethyl iodosilane. Journal of Molecular Structure, 2003, 644, 105-118.	3.6	5
83	Vibrational spectra, conformational equilibria, ab initio calculations and vibrational assignments of ethylmethylfluorosilane. Journal of Molecular Structure, 2006, 825, 101-114.	3.6	5
84	Conformational stability, r0 structural parameters, barriers to internal rotation, vibrational assignments and ab initio calculations of c-C3H5GeH2CH3. Journal of Molecular Structure, 2010, 969, 55-68.	3.6	5
85	The vibrational spectra of cis,cis-,trans,trans- and cis,trans-1,4-dichloro-1,3-butadiene. Spectrochimica Acta Part A: Molecular Spectroscopy, 1980, 36, 843-852.	0.1	4
86	The conformation and vibrational spectra of 2-ethynyl-1,3-butadiene (3-methylene-4-pentene-yne). Journal of Molecular Structure, 1987, 158, 249-257.	3.6	4
87	Conformational behaviour of five cyclobutane derivatives. Journal of Molecular Structure, 1988, 173, 389-396.	3.6	4
88	Vibrational spectra and conformations of 1,3-dibromo-2,2-dimethylpropane (DBDMP) and 2,2-di(fluoromethyl)-1,3-difluoropropane (TFN). Journal of Molecular Structure, 1988, 174, 259-266.	3.6	4
89	Vibrational spectra, conformations, ab initio calculations and vibrational assignments of 3-pentyn-2-ol. Journal of Molecular Structure, 2008, 879, 102-112.	3.6	4
90	FTi.r. (DRIFT-) investigation of glass-covered samples: Raman background and the acid strength of H-erionites. Zeolites, 1991, 11, 694-698.	0.5	3

#	Article	IF	Citations
91	Conformational stabilities, ab initio calculations and structural parameters for 2-chloroethyl silane and 2-chloroethyl trifluorosilane. Journal of Molecular Structure, 1999, 482-483, 385-389.	3.6	3
92	Vibrational spectra, quantum chemical calculations and spectral assignments of 1,1-difluoro-1-silacyclohexane. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 136, 51-57.	3.9	3
93	The vibrational spectra and conformation of 1,2-dicyanotetrafluoroethane. Spectrochimica Acta Part A: Molecular Spectroscopy, 1979, 35, 109-115.	0.1	2
94	The UV photolysis of azidomethane and 3-azidopropyne in nitrogen matrices. Journal of Molecular Structure, 1984, 115, 197-200.	3.6	2
95	Vibrational spectra and conformations of 1-chloro-4-fluorobut-2-yne. Journal of Molecular Structure, 1988, 174, 215-222.	3.6	2
96	The IR and Raman spectra and conformations of cyclohexyl azide. Journal of Molecular Structure, 1988, 174, 207-214.	3.6	2
97	The IR, Raman and NMR spectra and conformations of cyclohexylallene. Journal of Molecular Structure, 1990, 218, 59-66.	3.6	2
98	<title>Conformational equilibria and infrared matrix isolation spectra of bromoacetyl chloride and bromoacetyl bromide</title>. , 1992, , .		2
99	Vibrational spectra and conformation of 1-chloro-4-fluorobut-2-yne and ab initio calculations on 1,4-dihalobut-2-ynes. Journal of Raman Spectroscopy, 1992, 23, 167-180.	2.5	2
100	Ab initio Calculated Energies and Vibrational Frequencies of 3-Azidopropene (Allylazide)*. Zeitschrift Fur Physikalische Chemie, 1995, 191, 145-157.	2.8	2
101	The infrared and Raman spectra, conformations and ab initio calculations of 4-azidobut-1-yne. Journal of Molecular Structure, 1995, 349, 149-152.	3.6	2
102	Raman spectra,ab initiocalculations, phase transitions and conformations of 1,3-disilabutane. Phase Transitions, 2007, 80, 529-538.	1.3	2
103	Infrared and Raman spectra, conformations, ab initio calculations and spectral assignments of ethylmethyldichlorogermane. Journal of Molecular Structure, 2010, 976, 105-114.	3.6	2
104	The vibrational spectra and structure of diiminosuccinonitrile and N,Nâ€²-dichlorodiiminosuccinonitrile. Spectrochimica Acta Part A: Molecular Spectroscopy, 1980, 36, 29-36.	0.1	1
105	Vibrational spectra and conformations of 1, 4-dibromobut-2-yne and 1,4-diiodobut-2-yne. Journal of Raman Spectroscopy, 1992, 23, 391-400.	2.5	1
106	Spectra and structure of silicon containing compounds. Fresenius' Journal of Analytical Chemistry, 1995, 352, 499-507.	1.5	1
107	Infrared and Raman spectra, conformational stability, barriers to internal rotation, ab initio calculations and vibrational assignments for dichlorofluoroacetyl fluoride. Chemical Physics, 1997, 223, 131-148.	1.9	1
108	The shape of the ring in trans-1,3-dibromocyclobutane. Journal of Molecular Structure, 1997, 408-409, 455-458.	3.6	1

#	Article	IF	Citations
109	The vibrational spectra including matrix isolation, conformations and ab initio calculations of 4-azidobut-1-yne. Journal of Molecular Structure, 2000, 519, 101-117.	3.6	1
110	The infrared and Raman spectra of trans- and cis-tetrachloro-tetramethylbicyclopropylidene. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1166-1171.	3.9	1
111	Infrared and Raman spectral data and conformations of 1-pentyne. Journal of Molecular Structure, 2011, 989, 38-44.	3.6	1
112	Conformational Equilibria of Cyclohexylethene (Vinylcyclohexane) Investigated by Infrared and Raman Spectroscopy.. Acta Chemica Scandinavica, 1992, 46, 732-742.	0.7	1
113	The conformations and vibrational spectra of 2,2,4,4,6,6,9,9-octamethyl-3,7-decadiyne. Journal of Molecular Structure, 1987, 161, 63-73.	3.6	0
114	<title>FTIR studies of the reaction between atomic oxygen and CH3Br, CH2Br2, and CHBr3 in argon matrices</title>. , 1992, 1575, 335.		0
115	Vibrational spectra and conformations of 2-(Bromomethyl)-2-methyl-1,3-dibromopropane. Journal of Molecular Structure, 1992, 266, 289-294.	3.6	0
116	Vibrational spectra and conformation of 2,3-diiodobuta-1,3-diene. Journal of Raman Spectroscopy, 1993, 24, 299-302.	2.5	0
117	The vibrational spectra and conformations of 2,2-di (fluoromethyl)-1,3- difluoropropane. Journal of Molecular Structure, 1993, 293, 7-10.	3.6	0
118	Assay of the active ingredient of an MRI contrast agent using mid and near infrared spectroscopy and multivariate calibration. Journal of Molecular Structure, 1995, 348, 139-142.	3.6	0
119	The vibrational spectra and ab initio calculations of trans- and cis-1,3-dibromo-1,3-dimethylcyclobutane. Journal of Molecular Structure, 1997, 410-411, 471-475.	3.6	0
120	Conformational equilibrium in dimethylvinylsilane and dimethylvinylsilane-d1 studied by infrared and Raman spectroscopy and by ab initio calculations. Journal of Molecular Structure, 2003, 661-662, 81-107.	3.6	0
121	Vibrational spectra, conformational equilibrium, ab initio calculations and spectral assignments of ethylmethylgermane. Vibrational Spectroscopy, 2010, 54, 56-64.	2.2	0
122	Infrared and Raman spectra, DFT-calculations and spectral assignments of 1,1,3,3,5,5-hexafluoro-1,3,5-trisilacyclohexane. Journal of Molecular Structure, 2015, 1099, 399-406.	3.6	0
123	Conformational Studies by Vibrational Spectroscopy under High Pressure. , 1996, , 529-539.		0