EUROPEAN JOURNAL OF BIOMEDICAL AND PHARMACEUTICAL SCIENCES
http://www.ejbps.com

ISSN 2349-8870
Coden USA: EJBPBO
Volume: 13
Issue: 11
Year: 2026

EXPERIMENTAL (FTIR) AND AB INITIO AND DFT STUDY OF VIBRATIONAL FREQUENCIES OF AMINO ACID THREONINE

Santosh Kumar Srivastava[1]*, Vipin Bahadur Singh[2]

[1]Department of Physics, Singhania University, Pacheri Bari, Jhunjhunu (Rajasthan)-333515, India.
[2]Department of Physics, Udai Pratap (Autonomous) College, Varanasi-221002, India.

***Corresponding Author: Santosh Kumar Srivastava**

Department of Physics, Singhania University, Pacheri Bari, Jhunjhunu (Rajasthan)-333515, India.

DOI: https://doi.org/10.5281/zenodo.23804976

How to cite this Article: Santosh Kumar Srivastava[1]* and Vipin Bahadur Singh[2].(2026) Experimental (Ftir) And Ab Initio And Dft Study Of Vibrational Frequencies of Amino Acid Threonine. European Journal of Biomedical and Pharmaceutical Sciences, 13(11), 193–199.

This work is licensed under Creative Commons Attribution 4.0 International license.

Article Received on 01/10/2026 **Article Revised on 21/10/2026** **Article Published on 01/11/2026**

ABSTRACT
FTIR spectra of Threonine have been systematically analyzed using ab-initio and density functional theory calculations. The optimized geometries, harmonic vibrational wave numbers and intensity of vibrational bands of Threonine were calculated invoking different basis sets up to HF/6-311++G(d,p) and B3LYP/6-311++G(d,p) levels. Vibrational assignments have been made and calculated DFT frequencies and intensities of the Threonine at B3LYP/6-311++G(d,p) level are found to be in better agreement with corresponding experimental values in comparison to previous results.

KEYWORDS: Ab-initio, DFT calculations, FTIR spectra, Vibrational mode frequencies, Threonine.

1. INTRODUCTION

Threonine (2-amino-3-hydroxy-butanecarboxylic acid) is a member of aliphatic hydroxy amino acid. It is an important amino acid found in several proteins of human beings such as γ-globulin, β-lactoglobulin, hemoglobin, insulin, silk fibroin and among others.[1] Investigation of threonine is relevant for the physical point of view of both owing to the possibility to observe the behaviour of a system where the hydrogen bond plays a fundamental role[2-4] and the technological importance of a material which shows second harmonic conversion efficiency greater than 1 relative to potassium dihydrogen phosphate.[5] Requirements for Threonine appear to decrease with age and increase with stress. It is necessary for the formation of tooth enamel, elastin and collagen which are needed for both healthy skin and wound healing. Threonine also plays a role in preventing fat from accumulating in the liver. A fatty liver can affect liver function and is associated with diseases of the liver such as cirrhosis. Threonine has been investigated extensively by various authors.[6-11] Infrared (IR) absorption measurements and polarized Raman Scattering results for L-threonine at room temperature and assignments of some internal modes are also reported by Freire et al.[12] Schäfer and coworkers[7] considered gaseous threonine on the basis of favorable intramolecular interaction and yielded possible conformer. The ionization energies of four conformer of threonine has been calculated by Powis et al.[8] and compared with their synchrotron radiation photoelectron spectroscopy experiment. The orbital dependent vertical ionization energies of four threonine conformer have been studied by Dehareng et al.[9] using the outer valence green's function (OGVF) technique. Recently, the three hydroxy amino acids (serine, threonine and tyrosine) have been studied at the Hartree-Fock level of theory based on geometry optimization for one initial structure for each molecule by B. Lakard.[10]

However, a systematic study on the vibrational spectra and structure of threonine with the aid of ab-initio and DFT calculations (in the gas phase) up to higher basis sets using G-09 computer codes has been carried out. In the present work, ab initio and density functional theory calculations with B3LYP functional have been carried out using Gaussian-09 program [37] to estimate the optimized geometries, fundamental vibrational frequencies, intensities as well as the total energies of the

neutral threonine. The calculated vibrational mode frequencies of this species were compared with the observed frequencies in order to make more accurate vibrational assignments. A comparison of theoretical IR spectra and optimized geometry of threonine have also been made. In present study, electron correlation has been included using the DFT approximations with different basis sets. Density functional theory calculations are already reported to provide excellent agreement with experimental vibrational frequencies for organic compounds, if the calculated frequencies are scaled appropriately.[23-29]

2. METHODOLOGY

2.1 Experimental Study

Hydroxyamino acid (threonine) sample used in the present investigation was obtained from Merck (99% purity) have been used as such without further purification to record the infrared (IR) spectrum in a nujoll mull using a Fourier Transform IR spectrometer (JASCFTIR-5300) with a resolution of 2 cm^{-1} in the range of 400-4000 cm^{-1}. The IR spectrum of the molecule in a KBr pellet was also recorded on a Perkin Elmer RX1, FT-IR spectrometer in the range 450-4000 cm^{-1} with a resolution of 1 cm^{-1}.

2.2 Computational Methodology

The geometry optimizations and frequency calculations have been carried out with the Hartree-Fock[30] and density functional theory (DFT). Here, we have used the hybrid of Becke's non-local three parameter exchange and correlated functional with the Lee-Yang-Parr correlation functional (B3LYP) methods[31] using different basis sets viz; 6-311++G (d, p) and Aug-cc-pVDZ for the molecular orbital expansion without imposing any symmetry constraints. The optimized geometries at the B3LYP/6-311++G(d,p) level are used as starting geometry for optimization at the DFT/B3LYP/Aug-cc-pVDZ level of theory. The frequency calculations were carried out at same level as the respective optimization processes using analytic evaluation of the second derivatives of energy with respect to the nuclear displacement. The DFT/B3LYP method has been widely applied to obtain the conformational behavior, theoretical vibrational frequencies and infrared intensities of amino acids, which are well agreed with the experimental data for alanine[32], glycine[33], Proline[34], tyrosine[35] and valine.[36] All calculations in the present work were carried out using Gaussian 09[37] suite of ab initio quantum mechanical program.

3. RESULTS AND DISCUSSION

3.1 Geometry and Relative Energies

The optimized geometrical parameter (i.e. bond lengths, bond angles and dihedral angles) of hydroxyl amino acid (threonine) at RHF and DFT/B3LYP level of theories by employing 6-311++G(d,p) and Aug-cc-pVDZ basis sets in gas phase are listed in Table 1. The molecular structure of threonine is shown in Figure 1.

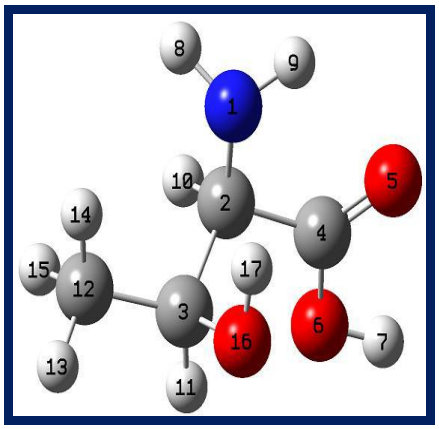


Fig. 1: Optimized Geometry of threonine at the DFT/B3LYP/6-311++G(d, p) level of theory.

Table 1: Geometrical Parameters of Threonine Using RHF and B3LYP methods by employing 6-311++G(d,p) and Aug-cc-pVDZ Basis Sets Respectively.

Geometrical parameters [a]	RHF		B3LYP	
	6-311++G(d, p)	Aug-cc-pVDZ	6-311++G(d, p)	Aug-cc-pVDZ
	Bond lengths (Å)			
N1-C2	1.451	1.453	1.463	1.464
N1-H8	0.997	0.999	1.011	1.014
N1-H9	0.999	1.001	1.015	1.017
C2-C3	1.541	1.540	1.556	1.555
C2-C4	1.518	1.518	1.523	1.522
C2-H10	1.090	1.095	1.099	1.104
C3-H11	1.082	1.086	1.091	1.097
C3-C12	1.524	1.524	1.529	1.529
C3-O16	1.399	1.403	1.420	1.422
C4-O5	1.183	1.189	1.206	1.212
C4-O6	1.324	1.328	1.350	1.353
O6-H7	0.946	0.948	0.969	0.971

C12-H13	1.084	1.089	1.092	1.097
C12-H14	1.086	1.090	1.094	1.099
C12-H15	1.087	1.092	1.095	1.100
O16-H17	0.945	0.946	0.970	0.972
	Bond angles (°)			
C2-N1-H8	112.2	111.9	112.4	112.2
C2-N1-H9	111.4	110.9	110.5	110.1
H8-N1-H9	109.1	108.8	109.0	108.7
N1-C2-C3	110.2	110.3	109.4	109.5
N1-C2-C4	109.3	109.2	109.2	109.2
N1-C2-H10	112.8	112.9	112.9	112.9
C3-C2-C4	110.9	110.9	111.3	111.3
C3-C2-H10	108.3	108.2	108.2	108.0
C4-C2-H10	105.3	105.2	105.9	105.8
C2-C3-H11	108.6	108.5	108.8	108.8
C2-C3-C12	112.0	112.0	111.6	111.6
C2-C3-O16	109.5	109.5	108.9	108.9
H11-C3-C12	108.9	108.9	109.5	109.5
H11-C3-O16	106.1	106.0	106.2	106.0
C12-C3-O16	111.6	111.6	111.7	111.7
C2-C4-O5	124.9	124.9	125.0	125.0
C2-C4-O6	112.3	112.5	112.1	112.2
O5-C4-O6	122.7	122.6	122.9	122.8
C4-O6-H7	108.9	108.4	107.4	107.0
C3-C12-H13	109.4	109.4	109.5	109.5
C3-C12-H14	111.3	111.2	111.0	111.0
C3-C12-H15	111.1	110.9	111.2	111.0
H13-C12-H14	108.0	108.1	107.9	108.1
H13-C12-H15	108.3	108.4	108.4	108.4
H14-C12-H15	108.7	108.7	108.7	108.8
C3-O16-H17	108.2	108.1	105.6	105.6
	Dihedral angles (°)			
H8-N1-C2-C3	-95.9	-94.6	-101.7	-101.5
H8-N1-C2-C4	142.0	143.2	136.3	136.4
H8-N1-C2-H10	25.2	26.6	18.8	18.9
H9-N1-C2-C3	141.5	143.7	136.3	137.3
H9-N1-C2-C4	19.4	21.5	14.3	15.2
H9-N1-C2-H10	-97.4	-95.1	-103.2	-102.3
N1-C2-C3-H11	-174.0	-174.8	-168.3	-168.8
N1-C2-C3-C12	65.6	64.9	70.8	70.2
N1-C2-C3-O16	-58.6	-59.5	-53.0	-53.6
C4-C2-C3-H11	-52.9	-53.6	-47.6	-47.9
C4-C2-C3-C12	-173.2	-173.9	-168.5	-168.9
C4-C2-C3-O16	62.5	61.7	67.7	67.3
H10-C2-C3-H11	62.2	61.3	68.3	67.9
H10-C2-C3-C12	-58.1	-59.0	-52.6	-53.1
H10-C2-C3-O16	177.6	176.6	-176.4	-176.9
N1-C2-C4-O5	-5.4	-6.19	-4.7	-5.1
N1-C2-C4-O6	176.9	176.3	176.8	176.5
C3-C2-C4-O5	-127.1	-127.9	-125.5	-126.1
C3-C2-C4-O6	55.2	54.5	55.9	55.5
H10-C2-C4-O5	116.0	115.2	117.2	116.8
H10-C2-C4-O6	-61.7	-62.3	-61.4	-61.6
C2-C3-C12-H13	179.7	179.3	-177.9	-178.3
C2-C3-C12-H14	-61.0	-61.4	-58.8	-59.1
C2-C3-C12-C15	60.2	59.8	62.4	61.9
H11-C3-C12-H13	59.6	59.2	61.6	61.1
H11-C3-C12-H14	178.8	178.6	-179.3	-179.7

H11-C3-C12-H15	-59.9	-60.3	-58.1	-58.6
O16-C3-C12-H13	-57.2	-57.4	-55.8	-56.1
O16-C3-C12-H14	62.1	61.9	63.3	63.1
O16-C3-C12-H15	-176.7	-176.9	-175.5	-175.8
C2-C3-O16-H17	51.9	51.7	46.8	46.6
H11-C3-O16-H17	168.9	168.6	163.8	163.6
C12-C3-O16-H17	-72.5	-72.9	-76.9	-77.1
C2-C4-O6-H7	-179.8	179.7	-179.5	179.9
O5-C4-O6-H7	2.4	2.1	1.9	1.5

[a] See Fig. 1 for the atom numbering.

In case of threonine, all the bond lengths increases, except the CC bond length as the basis set changed from 6-311++G(d,p) to Aug-cc-pVDZ at both level of calculations (See Table 1). The change in basis set does not change the CC bond lengths and it remains intact at both levels of theories. The bond angles of threonine found at the B3LYP/6-311++G(d,p) and B3LYP/Aug-cc-pVDZ levels are slightly less than the corresponding bond angles found at the RHF/6-311++G(d,p) and RHF/Aug-cc-pVDZ levels.

Total electronic energies with and without zero point energy corrections (ZPC), Rotational Constants, Dipole moments and Polarizabilities of hydroxy amino acid (threonine) using RHF and B3LYP methods by employing 6-311++G(d,p) and aug-cc-pVDZ basis sets are listed in Table 2.

Table 2: Total electronic energies (a.u.), Rotational Constants, Dipole moments and Polarizabilities of threonine using RHF and B3LYP methods by employing 6-311++G(d,p) and Aug-cc-pVDZ basis sets.

	RHF		B3LYP	
	6-311++G(d,p)	Aug-cc-pVDZ	6-311++G(d,p)	Aug-cc-pVDZ
Total electronic energies (a.u.)	-435.897448 (Without ZPC) -435.745532 (With ZPC)	-435.838784 (Without ZPC) -435.687258 (With ZPC)	-438.425267 (Without ZPC) -438.284285 (With ZPC)	-438.350257 (Without ZPC) -438.211864 (With ZPC)
Rotational constants				
A	3.20027	3.19212	3.12809	3.12083
B	1.51074	1.50992	1.47628	1.47373
C	1.31433	1.30953	1.29498	1.29169
Dipole moment (Debye)				
μ	3.0626	2.9576	3.0190	2.9138
Polarizabilities				
α_{xx}	66.348	70.361	77.282	81.368
α_{xy}	1.019	0.538	0.855	0.367
α_{yy}	60.826	63.770	69.905	72.896
α_{xz}	3.354	3.090	3.542	3.370
α_{yz}	2.738	2.416	2.420	2.150
α_{zz}	54.314	57.251	61.074	64.213

The total electronic energy of threonine with ZPC and without ZPC at DFT/B3LYP level of theory with 6-311++G(d,p) and Aug-cc-pVDZ basis set are found to be minimum than the corresponding total electronic energy with ZPC at the RHF level of theory with corresponding basis sets. Further, if we go from lower basis set i.e 6-311++G(d,p) to higher basis set i.e Aug-cc-pVDZ yields a decrease in the total electronic energy. Since there has been no experimental attempt to determine microwave spectra of gaseous threonine, the theoretically predicted rotational constants may be useful in searching gas phase conformers of threonine with microwave spectroscopy. Similarly, theoretically predicted dipole moments may assists experimentalist on the permanent dipole measurement. At both level of the theories RHF and B3LYP when we go from lower basis set to higher basis set, the dipole moments slight decreases in all the cases. This decrease is more at the B3LYP procedure which includes electron correlation than the RHF method. The polarizability tensor components also show a change in going from 6-311++G(d,p) basis set to Aug-cc-pVDZ basis set at both level of theories. In case of threonine xx, yy and zz component increases while xy, xz and yz component decreases. But they do not follow any regular pattern. The change in polarizability tensors xx, yy and

zz are more pronounced in all cases considered here at both level of theory.

3.2 Vibrational Characteristics

Vibrational frequencies of hydroxy amino acid (threonine) obtained through the IR spectrum are analyzed with the help of calculated frequencies using ab initio and DFT calculations. The Infrared spectrum has been taken between 400-4000 cm^{-1}. There are seventeen (17) atoms in the gaseous threonine molecule and having 45 vibrational modes. But, the vibrational modes below 400 cm^{-1} are not listed in the table for the sake of simplicity. The vibrational mode greater than 400 cm^{-1} i.e thirty seven (37) vibrational modes for threonine are listed in the corresponding Table 3. Table 3 shows the observed and theoretically calculated vibrational frequencies at the RHF and DFT level of theory by employing 6-311++G(d,p) and Aug-cc-pVDZ basis sets for the hydroxy amino acid threonine. The vibrational assignments for corresponding vibrational frequencies are also included in this table (See Table 3).

Table 3: Calculated and Experimental Fundamental Frequencies (cm^{-1}) of Threonine.

S. No.	Calculated frequencies				Expt. (IR) In nujoll mull (liquid)	Ref.[b]	Ref.[c]	Assignments
	RHF		B3LYP					
	6-311++G (d,p)	Aug-cc-pVDZ	6-311++G (d,p)	Aug-cc-pVDZ				
1	485 (3)	482 (2)	450 (4)	448 (4)	447	-	-	Φ
2	511 (69)	504 (98)	475 (28)	473 (29)	491	-	-	Φ
3	540 (97)	531 (61)	545 (22)	539 (32)	-	-	-	Tw of OH
4	583 (109)	579 (88)	574 (164)	558 (129)	560	-	-	Φ
5	678 (68)	672 (65)	630 (58)	625 (53)	-	-	-	Φ
6	705 (31)	700 (29)	659 (34)	654 (32)	-	-	-	Φ
7	794 (46)	792 (42)	728 (28)	725 (27)	747	-	-	Φ
8	909 (94)	908 (75)	830 (76)	828 (61)	-	-	-	WNH2
9	946 (11)	946 (12)	869 (24)	870 (25)	871	-	-	δ NH2
10	981 (80)	982 (75)	892 (77)	890 (65)	-	-	-	Φ
11	1022 (1)	1020 (1)	937 (1)	937 (1)	932	-	-	Φ
12	1110 (22)	1105 (20)	1026 (25)	1020 (21)	-	-	-	δ CH3
13	1184 (26)	1186 (42)	1076 (53)	1079 (55)	1040	-	1071	Tw CC
14	1192 (59)	1187 (43)	1104 (27)	1098 (23)	1093	-	-	Tw CC
15	1265 (131)	1262 (120)	1135 (154)	1136 (133)	-	-	-	ν CC
16	1284 (120)	1280 (102)	1162 (113)	1160 (110)	1185	-	1165	Tw CH
17	1337 (122)	1332 (134)	1221 (49)	1215 (59)	-	-	-	Tw NH2
18	1379 (17)	1378 (17)	1257 (21)	1251(18)	1246	-	-	Φ
19	1423 (11)	1419 (5)	1301 (3)	1293 (1)	-	-	1253	Tw CN
20	1468 (24)	1461 (16)	1336 (24)	1328 (19)	1318	-	-	δ CH
21	1495 (13)	1486 (10)	1369 (11)	1358 (10)	1347	-	1354	δ CH
22	1531 (9)	1519 (10)	1401 (5)	1385 (8)	1383	-	-	W CH3
23	1558 (56)	1546 (60)	1415 (23)	1410 (25)	-	-	-	Φ + δ CC
24	1567 (43)	1562 (41)	1430 (55)	1416 (59)	1418	-	1402	δ CH
25	1607 (8)	1590 (10)	1489 (6)	1466 (6)	1457	-	-	δ CH3
26	1620 (2)	1601 (2)	1501 (5)	1476 (5)	-	-	1478	δ CH3
27	1785 (73)	1767 (69)	1641 (77)	1623 (69)	1626	-	1656	W NH2
28	1994 (429)	1979 (396)	1807 (304)	1798 (282)	1651	-	1804	ν C=O of COOH
29	3152 (19)	3154 (22)	2999 (20)	3004 (20)	2873	-	-	ν_s C-H
30	3163 (32)	3167 (30)	3022 (23)	3028 (23)	2978	2974	-	ν_s C-H of CH3
31	3221 (23)	3232 (20)	3078 (2)	3090 (1)	2998	2912	2840	ν_s C-H
32	3240 (25)	3250 (26)	3094 (35)	3106 (36)	-	2989	2862	ν_s C-H2
33	3258 (46)	3266 (49)	3109 (23)	3121 (23)	-	-	2914	ν_{as} C-H2
34	3760 (15)	3754 (13)	3516(19)	3503 (17)	3026	3353	3397	ν_s N-H2
35	3845 (26)	3843 (24)	3611 (22)	3602 (21)	3169	3505	3469	ν_{as} N-H2
36	4117 (148)	4112 (138)	3712 (61)	3699 (55)	-	3600	3758	ν O16-H17
37	4123 (68)	4117 (62)	3762 (84)	3745 (79)	-	3686	3705	ν O6-H7 of COOH

[b]Ref.[10], [c]Ref.[11]

Vibrational spectra recorded in a nujoll mull. Numbers shown in the parenthesis correspond to the IR intensities. ν=Stretching, ν_{as}=Asymmetric stretching, ν_s= Symmetric stretching, δ=bending, δs= Symmetric bending, δas= Asymmetric bending, W = wagging, Sc= scissoring, Tw = twisting, T=torsion, Φ=deformation in molecule.

As we know that scaling varies with method and basis sets, and different scaling factors 0.8929 in RHF[37] and 1.0167 in DFT[38] are recommended in the literature. Even with these scaling, the calculated frequencies do not match well with the observed ones for two reasons. One reason is of course that the calculations refer to gas phase where hydroxy amino acid are neutral while the observation refers to zwitterionic form of amino acid. Another reason may be the small differences between the calculated and the observed geometrical parameters. Therefore scaling has been not carried out, although there is a good agreement (within 100 cm^{-1}) between observed and calculated frequencies. Also, the agreement is very well with other earlier reported vibrational frequencies for threonine. The three different spectral regions of the infrared spectrum of this hydroxy amino acid have been discussed below.

4000-2800 cm^{-1} region

In case of threonine the O-H stretching of carboxylic acid group and O-H stretching of alcohol group have been found at the 3745, 3699 and 1798 cm^{-1} at the DFT/B3LYP/Aug-cc-pVDZ level of theory (See Table 3). Our calculated stretching vibrational modes for O-H (carboxylic) and O-H (alcohol) are well agreed with earlier reported corresponding stretching vibrational modes by B. Lakard.[10] The stretching vibrational modes for NH2, CH3, CH, and CN are also in a good agreement with earlier reported corresponding stretching vibrational modes.[10,12] The NH2 stretching vibrations present in all amino acids. The asymmetric stretching of NH2 was observed at 3026 and 3169 cm^{-1} by Silva et al.[12], our calculated stretching modes of NH2 has been found at 3602 and 3503 cm^{-1} are higher than the observed ones by Silva et al. but well agreed with theoretically calculated by B. Lakard.[10] The CH vibration modes has been found from 3121 cm^{-1} to 3004 cm^{-1} at DFT/B3LYP/Aug-cc-pVDZ level of theory and in good agreement with observed ones 2882 cm^{-1} and 2932 cm^{-1} by Silva et al. as C-H stretching modes.

2000-1000 cm^{-1} region

In threonine, the theoretically calculated C=O stretching vibrational mode at the DFT/B3LYP level of theory with 6-311++G(d,p) and Aug-cc-pVDZ basis sets is found at the 1798 and 1807 cm^{-1} respectively and well agreed with C=O stretching mode reported by B. Lakard[10] (See Table 3). The bending mode of the CH3 has been found at the 1466 and 1476 cm^{-1} at the DFT/B3LYP level of theory with Aug-cc-pVDZ basis set. Bending vibrational mode of CH group has been found in between 1385 cm^{-1} to 1215 cm^{-1}.

1000-400 cm^{-1} region

The lower region of the IR spectrum of threonine molecule is complex in nature. The vibrational bands originates in this region are basically due to deformation in the skeleton of the molecule, deformation in the different functional groups, torsions in the different groups and mixing of different type of motions in the molecule.

4. CONCLUSION

The optimized geometries, harmonic vibrational wave numbers and intensities of vibrational bands of threonine were calculated at ab-initio and DFT levels invoking different basis sets up to 6-311++G (d,p) using G09 program. The structural parameters of threonine and the vibrational fundamentals from the IR spectra were analyzed and discussed with the help of the DFT calculations results in order to improve the previous assignments. We have re-investigated the effect of basis set in the optimized geometries and IR spectrum of threonine with the aid of high-level DFT calculations. It is clear that the geometrical parameters obtained for this amino acid are basis sets dependent. The addition of polarization function leads to longer bond length and shorter bond angles. The changes in different stretching vibrational modes of O-H groups have been analyzed.

REFERENCES

1. D. P. Shoemaker, J. Donohue, V. Schomaker, R. B. Corey, J. Am. Chem. Soc., 1950; 72: 2328.
2. Lautie, A. Novak, Chem. Phys. Letters, 1980; 71: 290.
3. V. A. Savelev N. D. Sokolov, Chem. Phys. Letters, 1975; 34: 281.
4. M. Falk, J. Raman Spectrosc., 1990; 21: 563.
5. K. E. Reickhoff, W. L. Peticolas, Science, 1965; 147: 610.
6. Pawlukojc, J. Leciejewicz, J. Tomkinson, S. F. Parker, Spectochim. Acta, A., 2001; 57: 2513.
7. L. Schäfer, S.Q. K. Newton, K. Siam, V. J. Klimokowski, C. Van. Alsenoy, J. Mol. Struct (Theochem)., 1990; 209: 373.
8. L. Powis, E. E. Rennie, U. Hergenhahn, O. Kugeler, R. B. Socrate, J. Phys. Chem. A., 2003; 107: 25.
9. D. Dehareng, G. Dive, Int. J.Mol. Sci., 2004; 5: 301.
10. B. Lakard, J. Mol. Struct. (Theochem)., 2004; 681: 183.
11. M. Zhang, Z. Lin, J. Mol. Struct. (Theochem)., 2006; 760: 159.
12. B. L. Silva, P. T. C. Freire, F. F. A. Melo, I. Guedes, M. A. Araujo Silva, J. Mendes Filho, A. J. D. Moreno, Brazilian J. of Phys., 1998; 28: 19.
13. R. C. Dunbar, J. Phys. Chem A., 2000; 104: 8067.
14. C. Ruan M.T. Rodgers, J. Am. Chem. Soc., 2004; 126: 14600.
15. H. F. Hameka, J. O. Jensen, J. Mol. Struct., 1993; 288: 9.
16. F. W. Teale, G. Weber, Biochem, J, 1957; 65: 476.
17. R. Ramaekers, J. Pajak, M. Rospenk, G. Maes, Spectrochimica Acta A, 2005; 61: 1347.

18. S.J. Martinez III, J.C. Alfano, D.H. Levy, J. M.ol. Spect.. 1992; 156: 421.
19. B. Kierdaszuk, L. Gryczynski, A.Modrak-Wojcik, A. Bzoska, D, Shugar, J.R. Lakowicz, Photochem. Photobiol., 1995; 61: 319.
20. J.R. Lakowicz, B. Kierdaszuk, P.Callis, H. Mallak, I. Gryczynski, Biophys. Chem., 1995; 56: 263.
21. S. Hill, US Army Research Lab. Adelphi, MD, Private Communication.
22. C Samuels, J. O. Jensen, H.F. Hameka, J. Mol. Struct. (Theochem)., 1998; 454: 25.
23. N. C. Handy, P.E. Maslen, R.D. Amos, J.S Andrews, C. W. Murray, G. Laming, Chem. Phys. Lett., 1992; 197: 506.
24. N. C. Handy, C.W. Murray, R.D. Amos, J. Phys. Chem., 1993; 97: 4392.
25. P. J. Stephens, F. J. Devlin, C. F. Chavalowski, M. J. Frish, J. Phys. Chem., 1994; 98: 11623.
26. F.J. Devlin, J.W. Finley, P.J. Stephens, M.J. Frish, J. Phys. Chem., 1995; 99: 16883.
27. S.Y.Lee, B.H.Boo, Bull. Korean Chem. Soc., 1996; 17: 754.
28. S.Y.Lee, B.H.Boo, Bull. Korean Chem. Soc., 1996; 17: 760.
29. A. Fu, D. Du, Z. Zhou, Spectrochim. Acta A., 2003; 59: 245.
30. W. J. Hehre, L. Radom, P.V.R. Schleyer, J. A. Pople, Ab initio Molecular Orbital Theory, Wiley, New York, 1986.
31. A. D. Becke, J. Chem. Phys., 1993; 98: 5648; C. Lee, W. Yang, R. G. Parr, Phys. Rev. B, 1988; 37: 785.
32. S. G. Stepanian, I.D. Reva, E.D. Radchenko, L.Adamowicz, J.Phys. Chem. A, 1998; 102: 4623.
33. S. G. Stepanian, I.D. Reva, E.D. Radchenko, M.T.S. Rosado, M. L. T. S. Duarte, R. F. L. Adamowicz, J. Phys. Chem. A, 1998; 102: 104.
34. S. G. Stepanian, I. D. Reva, E. D. Radchenko, L. A. damowicz, J. Phys. Chem. A, 2001; 105: 10664.
35. M. L. Zhang, Z. J. Huang, Z. J. Lin, J. Chem. Phys., 2005; 122: 134313.
36. S. G. Stepanian, I.D. Reva, E. D. Radchenko, L. Adamowicz, J. Phys. Chem. A, 1999; 103: 4404.
37. M. J. Frisch et al, Gaussian 09, Revision A.02, Gaussian, Inc. (Wallinford CT, 2009).
38. P. Scott and L. Radom, J. Phys. Chem., 1996; 100: 16502.