Science Advances Today

Sci. Adv. Today 2 (2016) 25261

Vibrational spectra, assignments, and normal coordinate analysis of hexachloroacetone

Sayyed Faramarz Tayyari*,†, Mahboobeh Gholamhoseinpour and Saeedreza Emamian

Department of Chemistry, Shahrood Branch, Islamic Azad University, Shahrood, Iran
† Permanent address: Chemistry Department, Ferdowsi University of Mashhad, Mashhad, Iran

*Author for correspondence: Sayyed Faramarz Tayyari, email: sftayyari@gmail.com

Received 16 Aug 2016, Accepted 17 Dec 2016, Published Online 17 Dec 2016

The FTIR and Raman spectra of 1,1,1,3,3,3-hexachloroacetone (HCA) have been recorded. The observed frequencies were assigned to the various modes of vibrations on the basis of normal coordinate analysis, assuming C_2 point group symmetry. The potential energy distribution associated with normal modes is also reported here. The fundamental vibrational frequencies calculated at the B2PLYP/6-31G(d) level agree well with the observed Raman and FTIR frequencies.

1. INTRODUCTION

1,1,1,3,3,3-Hexachloroacetone (HCA) is used in synthesis of many organic compounds [1-10] and its main use is as pesticide [11-15]. The structure of HCA has been studied by gas phase electron diffraction, *GED*, technique [16,17]. Andersen *et al.* [17] according to their *GED* study, concluded a C_1 symmetry point group for HCA molecule with two different ClCCO dihedral angles of 16.9º and 39.5º. However, Johansen *et al.* [16] concluded a C_2 structure for HCA with ClCCO dihedral angle of 31.6º. According to the Johansen *et al.* [16] results, the C=O, C-C, and C-Cl bond lengths are 1.184, 1.574, 1.764 Å, respectively. The measurements of dipole moments in the CCl_4 solution and as neat liquid of HCA give 1.24 and 1.34 Debye, respectively [18]. The energy of C_2 structure was 5.17 kcal/mol lower than the theoretical C_2v structure, calculated at the MP2/6-311+G(2d) level [16].

To the best of our knowledge, there is no report on the vibrational spectra of HCA in literature. Therefore, this study has been undertaken to record and study the FTIR and Raman spectra of HCA, and to assign the normal mode of vibrations on the basis of normal coordinate analysis.

2. METHODS

All geometry optimizations and vibrational spectroscopy calculations were performed using the Gaussian 09 package [19]. The optimized structures were further subjected to vibrational analysis at the same levels of theory. The vibrational modes were visualized by means of the GaussView program [20]. The calculated vibrational wavenumbers were compared with the observed Raman and FT IR data.

It has been shown in many theoretical calculations that the B3LYP level gives excellent results for vibrational analysis superior to all other DFT and HF approaches [21,22]. Therefore, the B3LYP level [23,24], using 6-311+G(p) basis set, was applied to calculate the vibrational wavenumbers of HCA. In order to obtain more accurate vibrational transition frequencies, anharmonic frequency calculations [25,26] were also performed at the aforementioned level of calculation. However, as the next section will show, this level is not very successful in predicting the vibrational wavenumbers of HCA with sufficient accuracy. On the other hand, it was shown that the B2PLYP level of theory [27,28], which combines the BLYP [23,29] functional with Hartree-Fock exchange and a perturbative second-order correlation part, is a promising functional for spectroscopic studies where a good accuracy of vibrational properties is required [30-32]. Consequently, the B2PLYP, using 6-31G(d) basis set, was also utilized for calculating the vibrational wavenumbers and their IR intensities and Raman activities.

The calculated Raman activities (R_A) were converted to relative Raman intensities (R_I) using the following relationship derived from the intensity theory of Raman scattering [34,35]:

$$I_{Ri} = \frac{f(\vartheta_0-\vartheta_i)^4 A_{R,i}}{\vartheta_i\left[1-exp\left(-\frac{hc\vartheta_i}{kT}\right)\right]} \qquad (1)$$

where ν_0 is the laser exciting wavenumber in cm^{-1} (ν_0 = 18789 cm^{-1} in this work, corresponding to 532 nm of the Nd:YAG laser), ν_i the vibrational wavenumber of the *i*th normal mode (cm^{-1}), while A_{Ri} is the Raman scattering activity of the normal mode ν_i. f (is a constant equal to 10^{-12}) is a suitably chosen common normalization factor for all peak intensities [35]. Symbols h, k, c, and T stand for Planck and Boltzmann constants, speed of light, and temperature in K, respectively.

A normal coordinate analysis was carried out to provide a complete assignment of the fundamental vibrational wavenumbers for HCA. The displacement internal coordinates were obtained from Gaussian outputs [36-39]. 31 standard internal coordinates containing 7 redundancies are defined as given in Table 1. From these internal coordinates, 24 non-redundant local symmetry coordinates were constructed by a suitable linear combination of internal coordinates (see Table 1). Then, all these symmetry coordinates were normalized through all 24 normal coordinates. The normalized symmetry coordinates were

© LOGNOR. All rights reserved.

Table 1. Internal and symmetric coordinates used to obtain vibrational normal modes of HCA[a].

Internal coordinates	Symmetry coordinates	Symmetry coordinates
R1=Δ(C1-O1)	νCO=R1	δCCC=2α3-α1-α2
R2=Δ(C1-C2)	νsCC=R1+R2	δCO=α1-α2
R3=Δ(C1-C3)	νaCC=R1-R2	γCO=Φ
ri=Δ(C-Cli)	νsCCl$_3$=(r1+r2+r3)±(r4+r5+r6)	τCF$_3$=ω1±ω2
α1=Δ(O-C1-C2)	νaCCl$_3$=(2x r1-r2-r3)±(2xr4-r5-r6)	
α2=Δ(O-C1-C3)	νa'CCl$_3$=(r2-r3)±(r5-r6)	
α3=Δ(C2-C1-C3)	δsCCl$_3$=(β1+β2+β3-γ12-γ13-γ23)± (β4+β5+β6-γ45-γ46-γ56)	
βi=Δ(C-C-Cli)	δaCCl$_3$=(2x γ23-γ12-γ13)±(2xγ56–γ45-γ46)	
γij=Δ(Cli-C-Clj)	δa'CCl$_3$=(γ12-γ13)±(γ45-γ46)	
Φ=Δ(OC1C2C3)	ρCCl$_3$=(β1-β2-β3)±(β4-β5-β6)	
ρi=Δ(Cli-C-C-O)	πCCl$_3$(β2-β3)±(β5-β6)	

a) ν, stretching; δ, deformation; τ, torsion; ρ, in-plane rocking; π, out-of-plane rocking; γ. out-of-plane bending.

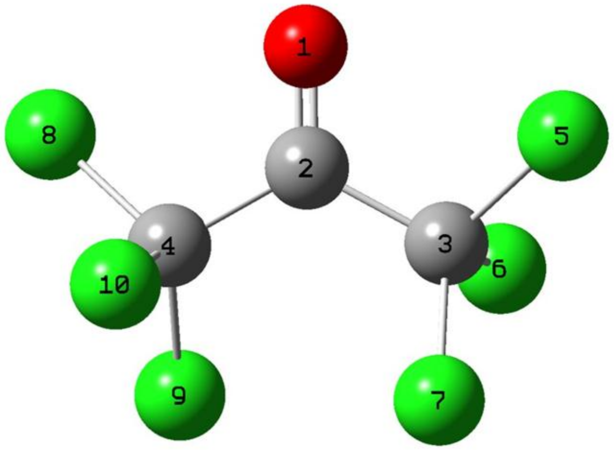

Figure 1. The optimized structure and atom numbering of HCA.

used to calculate the potential energy distributions (PED) for each normal mode. The "HP" keyword was applied in Gaussian calculations (using B2PLYP/6-31G(d) level) in order to obtain the high precision format (to five figures) for vibrational frequency eigenvectors (Cartesian displacement coordinates) printed in the frequency output of Gaussian 09 program [19]. All displacement coordinates (changes in bond lengths, bond angles, and dihedral angles), symmetry coordinates normalizations, and normal coordinate analysis calculations were carried out using the Microsoft® Excel 2013 program. The results of potential energy distribution (PED) in conjunction with the GaussView [20] program illustrations give the vibrational assignments with a high degree of accuracy.

3. EXPERIMENTAL PROCEDURES

Hexachloroacetone, HCA, was purchased from Sigma-*Aldrich chemical company*, *Germany*, and was used as such without further purification to record Raman and FTIR spectra.

The Raman spectrum of HCA has been recorded in the region 100 –1800 cm^{-1} on a Thermo Nicolet Almega dispersive Raman scattering spectrometer with a resolution of about 2 cm^{-1} operated with a 532 nm line from the second harmonic of a Nd:YLF laser in a backscattering configuration The laser power at the sample was 100 mW.

The FTIR spectra were recorded on a Bomem B-154 Fourier Transform spectrophotometer over the range 4000-450 *cm*$^{-1}$ by averaging 12 scans with a resolution of 2 cm^{-1}. The spectra were measured in the gas phase and as neat liquid. The liquid film was prepared by squashing a drop of HCA between two parallel KBr windows. A 10 cm pathlength gas cell with KBr windows was used for recording the gas phase IR spectrum.

4. RESULTS AND DISCUSSION

4.1. Geometry

The geometry and atom numbering of HCA is shown in Figure 1. The calculated and observed geometrical parameters of the titled molecule are listed in Table 1. As it is shown in this table, the geometrical parameters calculated at the B2PLYP/6-31G(d) level agrees fairly good with the experimental GED values reported by Johansen *et al.* [16]. The fully optimized structure, as resulted from GED study by Johansen *et al.* [16], belongs to the C_2 point group. According to GED studies reported by Johansen *et al.*, the HCA molecule, as hexafluoroacetone [37], belongs to the C_2 symmetry group with a ClCCO dihedral angle of 31.6º [16]. However, our calculations predict a value of about 23º for ClCCO dihedral angle of HCA molecule.

4.2. Harmonic and anharmonic vibrational frequencies

The harmonic and anharmonic vibrational frequencies calculated at the B3LYP/6-311+G(d) level and harmonic vibrational frequencies calculated at the B2PLYP/6-31G(d) level along with the experimental results for HCA are presented in Table 2. The complete assignments of fundamental vibrational band frequencies are also depicted in Table 2. The IR and Raman spectra of liquid HCA are shown in Figure 2 and 3, respectively.

According to the *C2* symmetry for the HCA molecule, the 3*N* − 6 = 24 vibrational modes can be classified among the symmetry species as follows:

$$\Gamma vib = 12A(\text{IR and R active}) + 12B(\text{IR and R active})$$

As shown in Table 2, while there is some disagreement between measured and calculated frequencies obtained with the B3LYP method, the calculated frequencies obtained with the B2PLYP level show excellent agreement with the observed results. A regression analysis shows a scaling for calculated frequencies obtained at the B2PLYP/6-31G(d) of 0.9845 (R^2= 0.99995 and standard deviation SD=5 cm^{-1}) and the corresponding value calculated by the B3LYP/6-311+G* level is 1.0067 (R^2= 0.99930 and standard deviation SD=19 cm^{-1}). These results indicate that the vibrational frequencies calculations performed at the B2PLYP level gives higher accurate wavenumbers for HCA molecule than B3LYP level.

This results indicate that the vibrational frequencies calculations performed at the B2PLYP gives very accurate wavenumbers for HCA molecule. The disability of B3LYP level of theory in predicting of vibrational frequencies of fluorinated compounds with high accuracy has

© LOGNOR. All rights reserved.

Table 2. Calculated and observed geometrical parameters of HCA[a].

	A	B	[16]	[17]
C=O	1.189	1.201	1.202(11)	1.201(14)
C-C	1.578	1.572	1.590(10)	1.597(5)
C-Cl5	1.785	1.778		
C-Cl6	1.806	1.796		
C-Cl7	1.786	1.779		
avgd.	1.792	1.784	1.772(3)	1.768(4)
dCCO	119.1	119.0	118.2(5)	118.3(9)
dCCC	121.9	122.0	123.5(11)	123.4(9)
dCCCl5	108.4	108.3		
dCCCl6	105.2	105.1		
dCCCl7	114.7	114.7		
avgd.	109.4	109.4	109.5(3)	-
Cl5-C-Cl6	109.3	109.5		
Cl5-C-Cl7	108.8	108.7		
Cl6-C-Cl7	110.4	110.5		
avgd.	109.5	109.6	109.5(3)	-
τ1	23.1	23.4	31.6±1.2	16.9±1.4
τ2	23.1	23.4		39.5±1.8
Symmetry	C2	C2	C2	C1
μ (Deby)	1.16	1.328	1.34 [18] 1.24	

[a] A, B3LYP/6-311+G(d); B, B2PLYP/6-31G(d); τ, dihedral angle

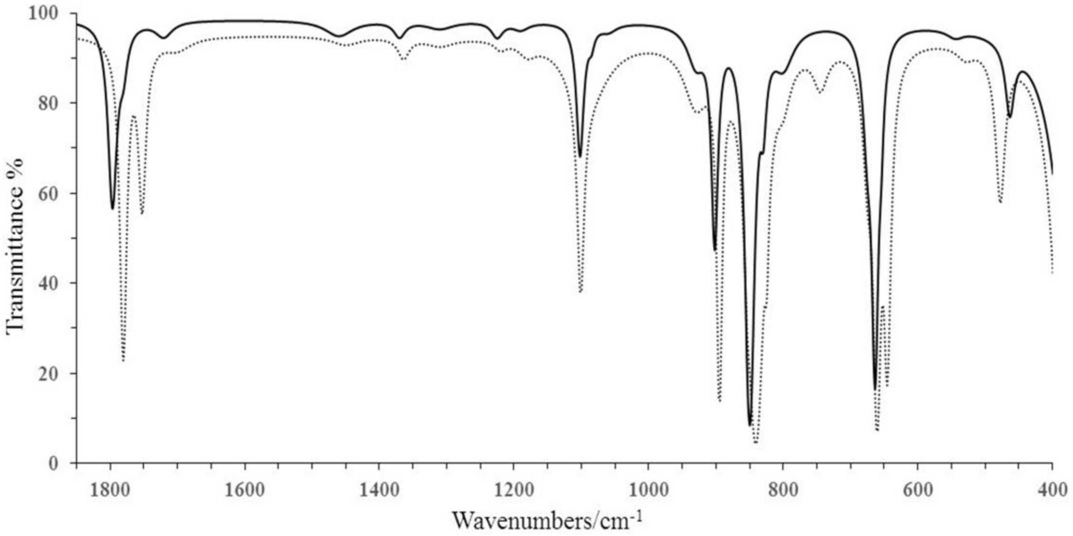

Figure 2. Gas phase (——) and neat liquid (·······) FTIR spectra of HCA.

been reported [37,38,40]. The scaled vibrational wavenumbers calculated at the B2PLYP/6-31G(d) level is also depicted in Table 2.

4.3. C=O group vibrations

Two bands are observed in both IR and Raman spectra at about 1780 and 1750 cm^{-1}. In the IR spectrum the former is very strong and the latter is a medium intensity band. The 1780 cm^{-1} band is unambiguously assigned to the C=O stretching vibration, ν1. The weaker band is considered as an overtone, 2ν2, which is in Fermi resonance with the ν1. As it is shown in Table 2, ν1 is mainly caused by C=O stretching, 43%. However, symmetric C-C stretching and C-C-C bending effectively contribute to this normal mode. On the other hand, symmetric C-C stretching and C-C-C bending highly participate in the ν2 normal mode. Therefore, the 1750 cm^{-1} band is most likely to be arisen from 2ν2, which is in strong Fermi resonance with ν1.

The C=O in-plane bending contributes in the ν13 (1100 cm^{-1}), ν15 (830 cm^{-1}), ν16 (663 cm^{-1}), ν18 (430 cm^{-1}), and ν19 (332 cm^{-1}) normal modes, with maximum contribution to the 430 cm^{-1} band. In acetone [39,41], the C=O in-plane bending mainly contributes in a band at 530 cm^{-1}.

The C=O out-of-plane bending has contributions in the ν14, ν15, ν16, ν17, ν21, and ν23 normal modes with the highest contribution in ν23, 160 cm^{-1}. In acetone [39] and hexafluoroacetone [37] the C=O out-of-plane bending mainly contributes in a band at 484 and 192 cm^{-1}, respectively.

© LOGNOR. All rights reserved.

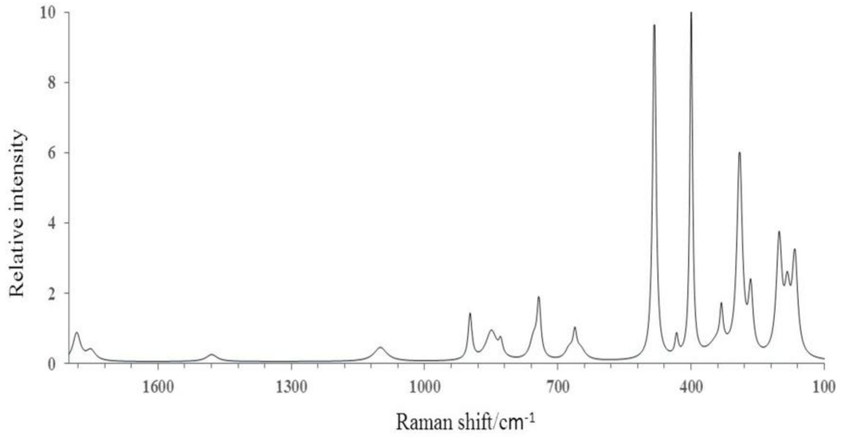

Figure 3. The Raman spectrum of neat liquid HCA.

Table 3. Calculated and observed fundamental vibrational frequencies (cm^{-1}) of HCA^{a}.

	F1	F2	I_{IR}	I_R	dpr	F3	F4	IR(gas)	IR(liq)	I_{IR}	R(liq)	I_R	
A													
ν1	1825	1795	34	12	0.41	1838	1812	1792	1780	vs	1785	w,p	νC=O(43) , νsC-C(21), δCCC(17), ρR(16)
								1762	1750	w	1750	vw,p	2x895=1790
ν2	910	895	56	19	0.75	880	862	892	895	sh	895	m,dp	νsR(31),δsR(25),νsCC(16),δCCC(23),ρR(12) δCCC(12), ρR(12)
ν3	865	851	66	3	0.09	831	816	846	845	vs	850	w,p	νaR(30), δsR(13),δaR(14), νsCC(11),νa’R(10)
ν4	746	734	1	37	0.63	697	682	-	745	vw	743	m,p	νa'R(37), δa’R(17) , νaR(12), πR(12)
ν5	476	468	6	97	0.06	462	459	469	475	m	481	vs,p	νaR(21), νsR(19) ,νa’R(12), νsCC(11),ρR(12)
ν6	405	398	1	100	0.02	394	390				400	vs,p	δsR(22), νsR(19), νaR(16), ρR(14)
ν7	299	294	0	87	0.75	292	289				291	s,dp	δa'R(39), δaR(39), νa’R(12) , πR(16)
ν8	270	266	0	41	0.74	265	262				266	m,dp?	δaR(34), δsR(16), δa’R(13)
ν9	206	203	0	68	0.52	201	199				201	m,p	δaR(18) , δsR(14), πR(14), ρR(14)
ν10	164	161	0	85	0.75	160	158				166	m,dp	πR(52), δa'R(13)
ν11	140	138	0	25	0.73	139	137						ρR(27), δaR(16), δa’R(15), νaR(10)
ν12	62	61	0	25	0.73	62	63						τR(100)
B													
ν13	1111	1093	17	4	0.75	1066	1047	1100	1098	s	1100	w,dp	νaC-C(40), δC=O(17) , ρR(11)
ν14	859	845	100	11	0.75	829	816	846	845		(850)		νa'R(29) , γCO(18), πR(18)
ν15	835	821	20	8	0.75	803	793	820sh	825	sh	829	vw,dp	νaR(21), δC=O(10), γCO(10)
ν16	673	662	87	10	0.75	652	642	661.5	663	vs	662	w,dp	νaR(20),δCO(14),γC=O(13), δsR(12),νsR(12)
ν17	645	634	54	4	0.75	621	609	640sh	647	s	650	sh,dp?	νa'R(28), γC=O(20)
ν18	432	425	2	1	0.75	422	417				430	vw,dp	νsR(24), δC=O(22), νaCC(15)
ν19	341	335	0	21	0.75	335	331				332	w,dp	δsR(27), δC=O(19), νaCC(10), δCCC(10)
ν20	290	285	1	87	0.75	282	279				(291)		δaR(25), νaR(12), νa’R(10) , νaCC(10)
ν21	280	275	0	17	0.75	274	271				(266)		δa'R(37) , δaR(19), γC=O(13), νa’R(10)
ν22	183	180	1	58	0.75	179	177				184	w,dp	ρR(25), νaCC(13), δaR(13), πR(12)
ν23	159	156	1	29	0.75	159	158						πR(28), γCO(22) , νCO(12)
ν24	30	30	1	38	0.75	33	34						τR(100)

[a] F1 and F2 stand for calculated unscaled and scaled (by 0.9835) wavenumbers at the B2PLYP/6-31G(d) level; F3 and F4 stand for calculated unscaled harmonic and anharmonic wavenumbers obtained at the B3LYP/6-311+G(d) level, respectively; I_{IR}, and I_R, stand for relative IR and Raman intensities, respectively; dpr, depolarization ratio; s, strong; w, weak; m, medium; ν, stretching; δ, bending; ρ, in plane rocking; π, out of plane rocking; a, asymmetric; a’, out of plane asymmetric; γ, out of plane bending; p, polarized; dp, depolarized; R, CCl_3 group; parentheses, band overlap.

© LOGNOR. All rights reserved.

4.4. CCl$_3$ groups vibrations

As shown in Table 2, the CCl$_3$ group vibrations contribute almost in all normal modes of HCA. The asymmetric CCl$_3$ stretching has high contributions to the ν13, ν3, ν14, ν4, ν17, and ν5 normal modes, which are observed at 1100, 846, 846, 743, 647, and 475 cm^{-1}, respectively. The symmetric CCl$_3$ stretching is significantly distributed over 910, 481, 430, and 400 cm^{-1} bands.

The symmetric CCl$_3$ deformation, δsCCl$_3$, contributes mainly to the 895, 400, and 332 cm^{-1} normal modes. An intense Raman band at 411 cm^{-1} has been attributed to the corresponding band for trichloromethyl chloroformate [42].

The asymmetric CCl$_3$ deformational modes contribute mainly in the ν7-ν9, ν20, and ν21 normal modes, which appear in the 290-200 cm^{-1} range. The CCl$_3$ rocking vibrations are mainly contributing to ν10, ν11, ν22, ν23, which appear in the 184-130 cm^{-1} range.

4.5. C-C vibrations

The symmetric CC stretching mainly contributes to the 1780, 895, and 840 cm^{-1} bands while the 1100 cm^{-1} band is mainly involved in the asymmetric CC stretching. The CCC bending vibrational mode predominantly contributes to the ν1(1780) and ν2 (895) cm^{-1} normal modes.

5. CONCLUSIONS

The vibrational spectra of HCA were completely assigned by using calculated harmonic and anharmonic vibrational wavenumbers performed at the B2PLYP and B3LYP levels. Excellent agreement exists between experimental and theoretical wavenumbers calculated at the B2PLYP/6-31G(d) level of theory. A normal coordinate analysis, using the eigenvectors calculated at the B2PLYP/6-31G(d), was performed for HCA. The theoretical calculations suggest a C$_2$ point group for HCA, which is consistent with the GED experimental results.

REFERENCES

1. R. T. Hrubiec, M. B Smith, J. Org. Chem. 49 (1984) 431.
2. S. Freedlander, T. A. Bryson, R. B. Dunlap, E. M. Schulman, C. A. Lewis Jr, J. Org. Chem. 46 (1981) 3519.
3. Bew, V. O. Joshi, J. Gray, P. T. Kaye, G. D. Meakins, J. Chem. Soc. Perkin Trans. 1 (1982) 945.
4. F. M. Laskovics, E. M. Schulman, J. Am. Chem. Soc. 99 (1979) 6672.
5. I. Yavari, M. Sabbaghan, Z. Hossaini, M. Ghazanfarpour-Darjani, Helv. Chim. Acta 91 (2008) 1144.
6. I. Yavari, M. Sabbaghan, Z. Hossaini, Monatsh. Chem. 139 (2008) 625.
7. I. Yavari, M. Sabbaghan, Z. Hossaini, Synlett 15 (2006) 2501.
8. M. Kulka, J. Am. Chem. Soc. 72 (1950) 1031.
9. R. M. Magid, O. S. Fruchey, W. L. Johnson, T. G. Allen, J. Org. Chem. 44 (1979) 359.
10. M. Harmata, Chem. Commun. 46 (2010) 8904.
11. R. Nadano, Y. Goto, US Patent, US Patent 6342640 (2002).
12. R. K. Mann, A. C. McVeigh-Nelson, US Patent, US Patent 8609588 (2013).
13. R. K. Mann, US Patent, US Patent 8680010 (2014).
14. N. N. Melnikov, Chemistry of Pesticides, Springer-Verlag, New York (1971).
15. A. H. Johnstone, In: R. C. Weast (Ed.), Handbook of chemistry and physics (1st Student Edition), CRC Press Inc., Boca Raton, Florida (1988) pp. ISBN0-8493-0740-6.
16. T. H. Johansen, S. Muren, K. Hagen, J. Mol. Struct. 567-568 (2001) 113.
17. P. Andersen, E. E. Astrup, A. Borgan, Acta Chem. Scand. A 28 (1975) 239.
18. R. K. Chan, Can. J. Chem. 47 (1969) 2253.
19. Frisch, M. J. , Trucks, G. W. , Schlegel, H. B. , Scuseria, G. E. , Robb, M. A. , Cheeseman, J. R. , Scalmani, G. , Barone, V. , Mennucci, B. , Petersson, G. A. , Nakatsuji, H. , Caricato, M. , Li, X. , Hratchian, H. P. , Izmaylov, A. F. , Bloino, J. , Zheng, G., Sonnenberg, J. L. , Hada, M. , Ehara, M. , Toyota, K., Fukuda, R. , Hasegawa, J. , Ishida, M. , Nakajima, T. , Honda, Y. , Kitao, O., Nakai, H. , Vreven, T. , Montgomery, J. A., Jr. , Peralta, J. E. , Ogliaro, F., Bearpark, M. , Heyd, J. J. , Brothers, E. , Kudin, K. N., Staroverov, V. N., Kobayashi, R. , Normand, J. , Raghavachari, K. , Rendell, A. , Burant, J. C., Iyengar, S. S. , Tomasi, J. , Cossi, M. , Rega, N. , Millam, J. M. , Klene, M., Knox, J. E. , Cross, J. B. , Bakken, V. , Adamo, C. , Jaramillo, J. , Gomperts, R. , Stratmann, R. E. , Yazyev, O. , Austin, A. J. , Cammi, R. , Pomelli, C., Ochterski, J. W. , Martin, R. L. , Morokuma, K. , Zakrzewski, V. G. , Voth, G. A. , Salvador, P. , Dannenberg, J. J. , Dapprich, S. , Daniels, A. D., Farkas, Ö., Foresman, J. B. , Ortiz, J. V., Cioslowski, J. , Fox, D. J., Gaussian 09 (Revision A. 02), Gaussian, Inc., Wallingford CT (2009).
20. GaussView (4. 1. 2), Gaussian Inc., Pittsburg, PA (2006).
21. J. Spanget-Larsen, Chem. Phys. 240 (1999) 51.
22. S. F. Tayyari, T. Bakhshi, S. Mehrani, E. R. Sammelson, J. Mol. Struct. 938 (2009) 76.
23. C. Lee, W. Yang, R. G. Parr, Phys. Rev. B 37 (1988) 785.
24. A. D. Becke, Phys. Rev. A 38 (1988) 3098.
25. V. Barone, J. Chem. Phys. 122 (2005) 014108.
26. V. Barone, J. Chem. Phys. 120 (2004) 3059.
27. S. Grimme, J. Chem. Phys. 124 (2006) 034108.
28. M. Korth, S. J. Grimme, J. Chem. Theory Comput. 5 (2009) 993.
29. A. D. Becke, J. Chem. Phys. 98 (1993) 5648.
30. V. Barone, M. Biczysko, J. Bloino, Phys. Chem. Chem. Phys. 16 (2014) 1759.
31. M. Biczysko, P. Panek, G. Scalmani, J. Bloino, V. Barone, J. Chem. Theory Comput. 6 (2010) 2115.
32. M. Biczysko, J. Bloino, C. Puzzarini, J. Chem. Phys. 141 (2014) 034107.
33. G. Keresztury, S. Holly, G. Besenyei, J. Varga, A. Wang, J. R. Durig, Spectrochim. Acta A 49 (1993) 2007.
34. G. Keresztury, Raman spectroscopy: Theory, In: J. M. Chalmers, P. R. Griffiths (Eds.), Handbook of Vibrational Spectroscopy Vol. 1, Wiley, Chichester (2001) p. 71–87.
35. P. B. Nagabalasubramanian, M. Karabacak, S. Periandy, Spectrochim. Acta A 85 (2012) 43.
36. F. Dolati, S. F. Tayyari, M Vakili, J. Mol. Struct. 1094 (2015) 264.
37. S. F. Tayyari, M. Golamhoseinpour, S. Emamiam, J. Fluorine Chem. 184 (2016) 65.
38. S. F. Tayyari, S. Holakoei, S. J. Mahdizadeh, J. Mol. Struct. 1041 (2013) 190.
39. M. Golamhoseinpour, S. F. Tayyari, S. Emamiam, Can. J. Chem. 94 (2016) 818.
40. S. F. Tayyari, F. Milani-Nejad, H. Rahemi, Spectrochim. Acta A 58 (2002) 1669.
41. H. Hollenstein, Hs. H. Günthard, J. Mol. Spectrosc. 84 (1980) 457.
42. V. B. Arce, C. O. Della Védova, A. J. Downs, S. Parsons, R. M. Romano, J. Org. Chem. 71 (2006) 3423.

Cite this article as:

Sayyed Faramarz Tayyari *et al.*: Vibrational spectra, assignments, and normal coordinate analysis of hexachloroacetone.
Sci. Adv. Today 2 (2016) 25261.

© LOGNOR. All rights reserved.