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Research Article

Calculation of the infrared spectrum of 4-Cyanostyrene by Hartree-Fock (HF) and Density Functional Theory (DFT)

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ABSTRACT

In this study, the molecular geometry of 4-Cyanostyrene molecule was optimized by using the Hartree–Fock (HF) and density functional theory (DFT/B3LYP) with 6-311G(d,p) basis set in the ground state. After the optimization, infrared vibration bands of 4-Cyanostyrene molecule were calculated by using the Hartree–Fock (HF) and density functional theory (DFT/B3LYP) with 6-311G(d,p) basis set. The theoretically calculated vibrational frequencies were multiplied by a scalar factor to correlate to experimental results. These theoretically obtained frequencies were compared exactly with the experimental results of 4-Cyanostyrene. All calculated frequencies were discussed. Finally, the correlation graphs of the theoretical and experimental results were obtained. The results were seen to be quite compatible with each other.

Keywords: 4-Cyanostyrene, Harteree-Fock (HF), density functional theory (DFT), infrared (IR).

4- Siyanostirenin infrared spektrumunun Hartree-Fock (HF) ve yoğunluk fonksiyon teorisiyle (DFT) hesaplanması

ÖZ

Bu çalışmada, 4-Siyanostiren molekülünün temel halde moleküler geometrisi, Hartree-Fock (HF) ve 6-311G (d, p) temel sete sahip yoğunluk fonksiyonel teorisi (DFT/B3LYP) kullanılarak optimize edildi. Optimizasyondan sonra 4-Siyanostiren molekülünün infrared titreşim bantları, Hartree-Fock (HF) ve 6-311G (d, p) temel sete sahip yoğunluk fonksiyonel teorisi (DFT/B3LYP) kullanılarak hesaplandı. Teorik olarak hesaplanan titreşim frekansları, deneysel sonuçlarla ilişkilendirmek için bir skale faktör ile çarpıldı. Teorik olarak elde edilen bu frekanslar, 4-Siyanostirenin deneysel sonuçlarıyla tam olarak birebir karşılaştırıldı. Hesaplanan tüm frekanslar tartışıldı. Son olarak teorik ve deneysel sonuçların korelasyon grafikleri elde edilidi. Sonuçların birbiriyle oldukça uyumlu olduğu görüldü.

Anahtar Kelimeler: 4-siyanostiren, Harteree-Fock (HF), yogunluk fonksiyon teorisi (DFT), kızılötesi (IR).

1. INTRODUCTION

Styrene is most commonly found in cigarette smoke, polluted atmosphere and working areas. Styrene and styrene-7,8-oxide are used in plastic reinforcement and rubber industry. Styrene-7,8-oxide molecule is the basic metabolite of styrene in the human body.[1] Many researchers have revealed that styrene and styrene-7,8-oxide substances cause various cancers, and increase risk of cancer in groups working in the plastics industry.[2-10] Styrene model is studied on the rotation of a vinyl group attached to the benzene ring. Thus, many scientists have worked on this topic. Hollas and co-workers have accepted the structure of styrene as planar and determined its vibrations with the help of the electronic absorption spectrum.[11] Zilberg and Haas have studied the fluorescence spectra of the styrene, and also they have investigated trans-β-methyl styrene substances in both the ground state and twice-excited state, finally carried out the theoretical ab initio study.[12] The rotational constant of the vinyl group in the planar structure of the styrene has been calculated by Bock and co-workers based on ab initio calculations.[13] In the literature, although there are many experimental and theoretical studies about styrene and trans-β-methyl

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styrene, it is seen that 4-Cyanostyrene, a derivative of styrene, has not been studied both experimentally and theoretically. Therefore, in this study, it is aimed to calculate the infrared vibration frequencies of the planar 4-Cyanoster molecule using HF and DFT methods.

2. CALCULATIONS

Infrared vibration calculations were carried out using the Gaussian 09 software on a windows system.[14] As mentioned above, the shape of the molecule was considered as plane, and the input data was created by using Gauss View molecular visualization program.[15] The data created above was reused in HF/6-311G (d, p) and DFT/B3LYP/6-311G (d, p) to find optimization, that is, the lowest energy level of the molecule. In this case, bond lengths, bond angles and dihedral angles in the molecule were calculated. Thus, by optimizing the molecule, negative vibrations were prevented. All the vibration frequencies in the basic state of the molecule were obtained using the same HF/6-311G (d, p) and DFT/6-311G (d, p) calculation methods. The theoretically calculated number of vibrations is considerably greater than that observed experimentally. This means that the compound is large and the calculations are done in gas phase. Since the 4-Cyanostyrene molecule is planar and has a C_s symmetry, all vibrations are both raman and infrared active. Considering the method mentioned above, a total of 45 vibrations were calculated as 31 in-plane (A') and 14 out-of-plane (A"). The frequencies obtained were multiplied by scalar factors of 0.9085 and 0.9669, respectively. All the frequencies are assigned in terms of fundamental, overtone and combination bands. As shown in Figure 1, the 4-Cyanostyrene molecule has 17 atoms.

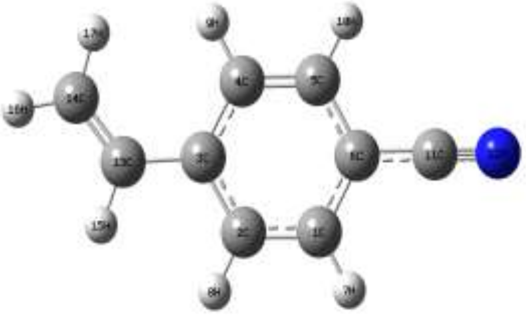


Figure1. 4-Cyanostyrene molecule.

3. RESULTS AND DISCUSSION

3.1. Combination and overton bands

The experimental infrared vibrational spectra of 4-Cyanostyrene molecule are shown in Figure 2.[16]

The infrared vibration frequencies obtained from the calculations and the experimental data are given in Table 1. As seen in Figure 2, the bands between 2100 cm^{-1} - 1700 cm^{-1} are the combinations of the benzene ring. For example, in Figure 2, the band at 1846 cm^{-1} is determined as the sum of the 536 cm^{-1} and 3100 cm^{-1} bands. The bands between 3100 cm^{-1} - 4000 cm^{-1} are the overtone bands. The band at 3392 cm^{-1} is designated as the overtone band, which is four times the 848 cm^{-1} band.

3.2. Vinyl group vibrations

Asymmetric and symmetric C-H stretch vibrations in the vinyl group appear between the regions 3090 cm^{-1} - 3075 cm^{-1} and 3050 cm^{-1} - 3000 cm^{-1}, respectively.[17] The 3090 cm^{-1} band observed in the spectrum was marked as asymmetric C-H stretch and was calculated as 2991.3675 cm^{-1} in HF and 3120.3907 cm^{-1} in DFT. Symmetrical C-H stress vibration at the spectrum was observed at 3012 cm^{-1} and calculated as 2861.8122 cm^{-1} in HF and 342.5710 cm^{-1} in DFT. The C-H tensile vibration band in vinyl appears around 3000 cm^{-1}.[18] Looking at the spectrum, this band was observed at 2994 cm^{-1} as medium and was calculated as 2839.0217 cm^{-1} in HF and 3033.3085 cm^{-1} in DFT. The calculation of HF deviated from the experimental value by approximately 150 cm^{-1}. In general, in the infrared spectrum, C = C tensile vibration bands of vinyl, vinylidine and cis alkenes are observed in the range of 1600 cm^{-1} to 1635 cm^{-1}.[17] However, this C = C tensile vibration band was observed at 1627cm^{-1} with medium intensity. This band was calculated as 1677.4357 cm^{-1} in HF and 1634.5753 cm^{-1} in DFT.

In-plane bending vibrations of the vinyl molecule appear between 1075 cm^{-1} and 1415 cm^{-1}.[18] In the spectrum, the band observed at 1423 cm^{-1} with medium intensity was marked as symmetrical in-plane bending (scissoring) vibration of the CH_2 group in vinyl. In Figure 2, the band that appears to be rather weak at 1310 cm^{-1} was marked as the C-H in-plane bending vibration. The band observed at 1014 cm^{-1} with medium intensity was marked as rocking in the plane. It is understood from Table 1 that these three bands marked are in harmony with the calculated values.

The out-of-plane C-H bending vibrations in the vinyl group are generally observed in the range of 985cm^{-1} to 915 cm^{-1}.[17] A closer look at the spectrum revealed that the band at 991 cm^{-1} was very intense and marked as out-of-plane C-H bending vibration. Likewise, the band which was observed to be very strong at 922 cm^{-1} was marked as out-of-plane wagging. It is understood from Table 1 that these bands are in agreement with the theoretically calculated results. As a consequence, these values are compatible with many experimental and theoretical results.[19-26]

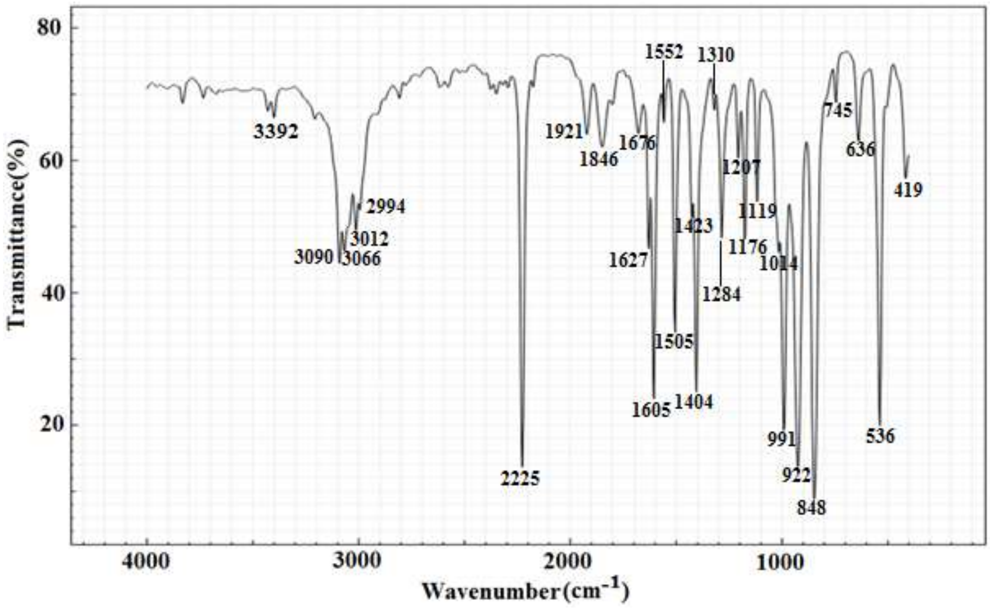


Figure 2. The experimental infrared vibrational spectra of 4-Cyanostyrene molecule.

3.3. C≡N vibrations

In the infrared spectrum, C≡N tensile vibration bands of benzonitriles between 2220 cm^{-1} and 2240 cm^{-1} are observed to be strong. This C≡N stretch band may slide higher or lower depending on the condition of the groups attached to the benzene ring.[27-29] Looking at the infrared spectrum, it was observed as a very strong at 2225 cm^{-1}, and it was assigned as C≡N strain vibration. The peak observed at 536 cm^{-1} was marked as the C-N out-of-plane bending band. From Table 1, it seems that the experimental results and the theoretical results are highly compatible with each other.

3.4. Ring vibrations

3.4.1. C-H vibrations

The peaks observed between 3000-3100 cm^{-1} are aromatic C-H tensile vibrations[30] and they are pure. Looking at the spectrum, the peak that appear at 3066 cm^{-1} with medium intensity was marked as aromatic C-H stretch band. This peak was calculated at 2873.7293 cm^{-1} in HF and 3066.5823 cm^{-1} in DFT. In-plane and out-of-plane C-H bending vibrations are observed at 1000-1300 cm^{-1} and 950-800 cm^{-1}, respectively.[31-33] Looking at the spectrum, the bands observed at 1284 cm^{-1}, 1207 cm^{-1}, 1176 cm^{-1} and 1119 cm^{-1} at medium intensity were marked as in-plane bending. These bands were calculated as 1315.5468 cm^{-1}, 1216.6726 cm^{-1}, 1197.0028 cm^{-1} and 1078.4971 cm^{-1} in HF and 1284.7295 cm^{-1}, 1191.5421 cm^{-1}, 1189.9749 cm^{-1} and 1104.8523 cm^{-1} in DFT, respectively. However, as seen in Table 1, it can be said that the calculated HF values deviate slightly from the experimental values. The band that appears to be very strong at 848 cm^{-1} in the spectrum is marked as out-of-plane bending and is compatible with DFT calculation.

3.4.2. C-C vibrations

In the infrared spectrum, aromatic C-C stretch vibrations generally occur between 1620 cm^{-1} and 1400 cm^{-1}.[17] Looking at the spectrum, the bands at 1627 cm^{-1}, 1605 cm^{-1}, 1552 cm^{-1}, 1504 cm^{-1}, 1423 cm^{-1} and 1404 cm^{-1}, which appear to be strong and very weak in this range, were marked as C-C ring strain vibrations. The bands observed very weak at 745 cm^{-1} and medium strength at 419 cm^{-1} were marked as out-of-plane C-C bending vibration. From Table 1 these signs seem to agree with the theoretical results.

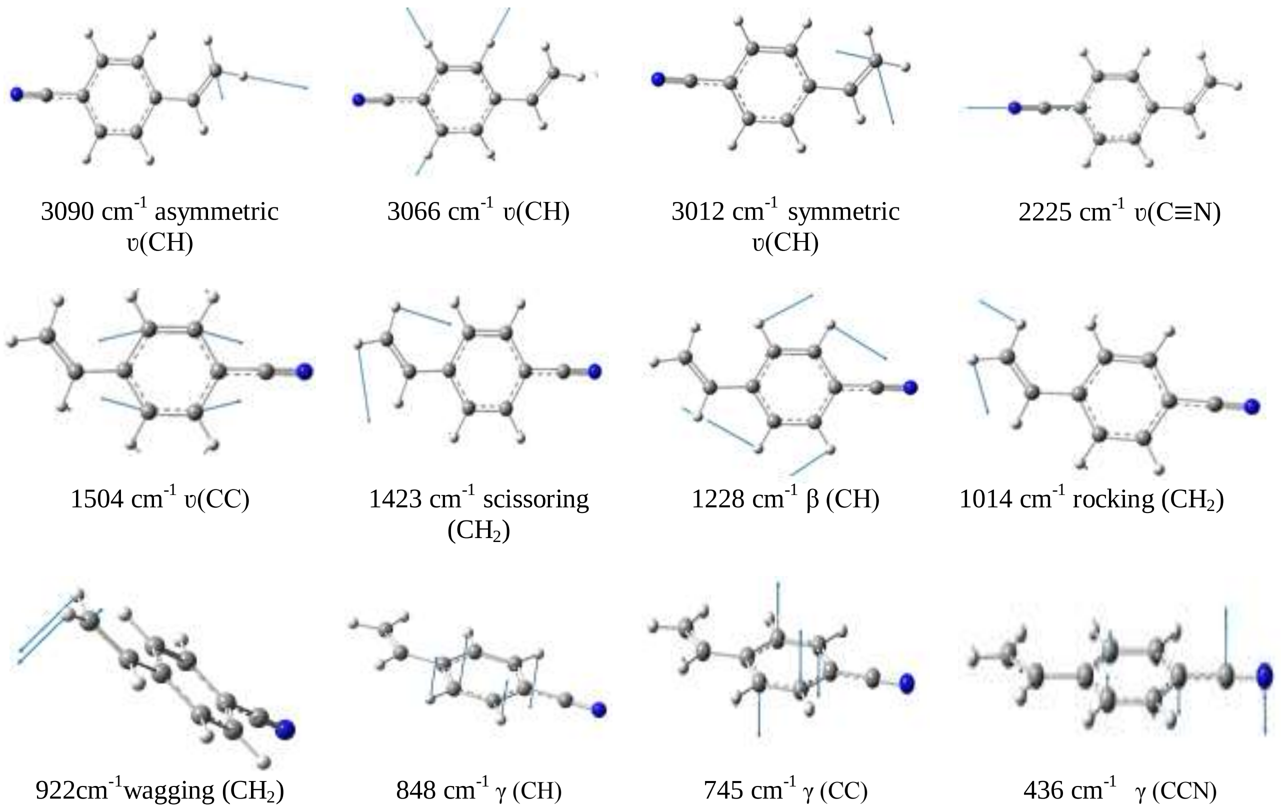
Although the observed bands are compatible with the literature, there is some difference in calculation. This may be due to the calculation of the molecule in the gas phase. It is also known from the literature that the frequencies calculated by the HF method are higher than other methods.[34,35]

Table 1. Frequencies obtained from the calculations and the experimental data along with their assignment

		Calculation HF/6-311G(dp)			**Calculation DFT/B3LYP/6-311G(dp)**				
N	T	Frequency	IR Int.	Scaled[a]	Frequency	IR Int.	Scaled[b]	Exp.[c]	Assignment
1	A"	67.1829	0.6598	61.0356	28.7136	0.3670	27.7631	--------	(C_2H_3) torsion
2	A"	207.0090	1.3737	188.0676	103.7538	1.3654	100.3195	--------	Butterfly
3	A'	217.6998	4.3485	197.7802	141.2461	4.3033	136.5708	--------	β (C_2H_3)+ β (C≡N)
4	A"	337.7575	4.0868	306.8526	244.7321	4.3430	236.6314	--------	Fluctation
5	A'	354.4086	2.2227	321.9802	245.4644	1.2741	237.3395	--------	β (C_2H_3)
6	A'	418.7019	0.5483	380.3906	384.9904	0.3762	372.2472	--------	υ molecule
7	A"	472.9675	0.0651	429.6909	408.4511	0.2545	394.9313	--------	γ (CCH)
8	A"	524.9858	1.4553	476.9495	426.7356	4.0108	412.6106	419 m	γ (CCH)
9	A'	581.2008	4.7494	528.0209	511.2766	2.9985	494.3533	--------	β (CH_2)
10	A"	653.8436	15.9323	594.0169	559.0377	18.8979	540.5335	536 s	γ (CCN) at Cy.
11	A'	655.5855	0.5163	595.5994	574.3667	0.2203	555.3551	--------	β (CCN) at Cy.
12	A"	721.9496	0.3528	655.8912	655.1946	3.3536	633.5076	--------	γ (CCH)
13	A'	751.8163	0.1759	683.0251	662.7756	0.1241	640.8377	--------	Ring Deformation
14	A'	752.0514	2.3801	683.2386	685.7267	0.0990	663.0291	--------	Molecule Deformation
15	A"	861.3360	1.0637	782.5237	770.4318	0.0814	744.9305	745 vw	γ (CCH)
16	A'	891.5065	1.7953	809.9336	826.4174	0.3285	799.0629	--------	Ring Deformation
17	A"	1023.1287	57.4272	929.5124	846.6817	0.8861	818.6565	--------	γ (CH) at ring
18	A"	1031.7333	0.1472	937.3297	867.8710	48.0671	839.1444	848 vs	γ (CH) at ring
19	A"	1114.0998	0.3477	1012.1596	945.3533	42.3555	914.0621	922 vs	CH_2 Wagging
20	A"	1127.8882	46.5517	1024.6864	977.8831	0.4127	945.5151	--------	γ (CH) at ring
21	A"	1151.3583	3.6369	1046.0090	982.7572	0.0812	950.2279	--------	γ (CH) at ring
22	A"	1151.8021	1.2139	1046.4122	1028.8205	16.1885	994.7665	991 vs	γ (CH) at V.
23	A'	1166.6827	0.3499	1059.9312	1033.1801	2.5824	998.9818	--------	Ring breathing
24	A'	1181.7350	21.5229	1073.6062	1049.6640	4.9647	1014.9201	1014 m	CH_2 Rocking
25	A'	1187.1185	3.4969	1078.4971	1142.6749	3.6784	1104.8523	1119 m	β (CH) at ring
26	A'	1283.8421	5.2075	1166.3705	1199.4351	3.2776	1159.7337	--------	υ C-(C≡N)
27	A'	1317.5596	5.5843	1197.0028	1230.7115	1.1041	1189.9749	1176 m	β (CH) at ring
28	A'	1339.2104	4.7716	1216.6726	1232.3323	0.3595	1191.5421	1207 w	β (CH) at ring
29	A'	1359.1966	2.7419	1234.8301	1315.2104	5.7635	1271.6769	--------	β (CH) at V.
30	A'	1448.0428	2.9391	1315.5468	1328.7098	0.2190	1284.7295	1284 m	β (CH) at ring
31	A'	1484.8981	0.0234	1349.0299	1355.5765	0.8538	1310.7069	1310vw	β (CH) at V.
32	A'	1566.5226	16.8539	1423.1857	1438.4795	11.8529	1390.8658	1404 s	υ(CC) at ring
33	A'	1612.0305	4.5415	1464.5297	1462.0319	2.9805	1413.6386	1423 m	(CH_2) Sc. + υ(CC) at ring
34	A'	1693.7875	25.2312	1538.8059	1540.0096	14.3853	1489.0352	1504 s	υ(CC)at ring
35	A'	1739.4688	3.4180	1580.3074	1589.3371	1.1049	1536.7300	1552vw	υ(CC) at ring
36	A'	1801.0285	42.9698	1636.2343	1649.0936	18.7440	1594.5086	1605 s	υ(CC) at ring
37	A'	1846.3795	3.6552	1677.4357	1690.5320	4.7590	1634.5753	1627 m	υ(C=C)atV.+υ(CC)at ring
38	A'	2446.3422	95.5720	2222.5018	2335.1359	46.0782	2257.8429	2225 vs	υ(C≡N)
39	A'	3124.9551	4.6786	2839.0217	3137.1482	13.3434	3033.3085	2994 m	υ(CH) at V.
40	A'	3150.0410	9.2565	2861.8122	3146.7277	3.2470	3042.5710	3012 m	S. υ(CH) at V.
41	A'	3163.1583	17.6060	2873.7293	3171.5610	9.0007	3066.5823	3066 m	υ(CH) at ring
42	A'	3183.5435	5.6943	2892.2492	3184.2780	3.7021	3078.8783	--------	υ(CH) at ring
43	A'	3185.6607	7.1484	2894.1727	3197.9466	6.8913	3092.0945	--------	υ(CH) at ring
44	A'	3204.7402	10.0409	2911.5064	3200.2597	1.9608	3094.3311	--------	υ(CH) at ring
45	A'	3292.6445	14.5605	2991.3675	3227.2114	10.7017	3120.3907	3090 m	A. υ(CH) at V.

Scaled[a]: 0.9085, scaled[b]: 0.9669, A.: asymmetric, A': in-plane, A": out-of-plane, Sc.: scissoring, S.: symmetric, Cy.: cyano, V.: vinyl, υ: in plane stretch, β: in plane bending, γ: out of plane bending, T: type, N: number, c: Ref.16.

Some vibration types of the 4-Cyanostyrene molecule are listed in Figure 3.



3090 cm^{-1} asymmetric υ(CH)

3066 cm^{-1} υ(CH)

3012 cm^{-1} symmetric υ(CH)

2225 cm^{-1} υ(C≡N)

1504 cm^{-1} υ(CC)

1423 cm^{-1} scissoring (CH_2)

1228 cm^{-1} β (CH)

1014 cm^{-1} rocking (CH_2)

922cm^{-1}wagging (CH_2)

848 cm^{-1} γ (CH)

745 cm^{-1} γ (CC)

436 cm^{-1} γ (CCN)

Figure 3. Vibration types of the 4-Cyanostyrene molecule.

4. CONCLUSIONS

The IR frequencies and intensities of the fundamental vibrational bands of 4-Cyanostyrene were calculated using HF and DFT/B3LYP methods with 6–311G(dp) basis set. The infrared absorption and intensities, computed by B3LYP method, are in reasonable agreement with the experimental data. The results confirm the ability of the methodology applied for interpretation of the vibrational spectrum of the 4-Cyanostyrene molecule in the solid state. It is important to do such a study first time on the 4-Cyanostyrene molecule.

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Conflict of interests

Authors declare that there is no a conflict of interest with any person, institute, company, etc.

REFERENCES

1. Rappaport, S. M.; Yeowell-O'Connell, K.; Bodell, W.; Yager, J. W.; Symanski, E. *Cancer Res.* **1996**, 56 (23), 5410-5416.

2. Kogevinas, M.; Ferro, G.; Andersen, A. et al. *Scand. J. Work Env. Hea.* **1994**, 20 (4), 251-261.

3. Coggon, D.; Ntani, G.; Harris, E. C.; Palmer, K. T. *Occup. Environ. Med.* **2015**, 72 (3)**,** 165-170.

4. Christensen, M. S.; Vestergaard, J. M.; d'Amore, F. et al. *Epidemiology* **2018**, 29 (3), 342-351.

5. Collins, J. J.; Bodner, K. M.; Bus, J. S. *Epidemiology* **2013**, 24 (2), 195-203.

6. Nissen, M. S.; Stokholm, Z. A.; Christensen, M. S.; Schlünssen, V.; Vestergaard, J. M.; Iversen, I. B.; Kolstad, H. A. *Occup. Environ. Med.* **2018**, 75 (6), 412-414.

7. Cruzan, G.; Bus, J. S.; Banton, M. I.; Sarang, S. S.; Waites, R.; Layko, D. B.; Raymond, J.; Dodd, D.;

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Andersen, M. E. *Toxicol. Sci.* **2017**, 159 (2), 413-421.

8. Cruzan, G.; Cushman, J. R.; Andrews, L.S.; et al. *J. Appl Toxicol.* **2001**, 21 (3), 185–198.

9. Ponomarkov, V.; Tomatis, L. *Scand. J. Work Environ. Hea.* **1978**, 4 (2)**,** 127–135.

10. Conti, B.; Maltoni, C.; Perino, G.; Ciliberti, A. *Ann. NY Acad. Sci.* **1988**, 534 (1), 203-234.

11. Hollas, J. M.; Khalilipour, E.; Thakur, S. N. *J. Mol. Spectrosc.* **1978**, 73 (2), 240-265.

12. Zilberg, S.; Haas, Y. *J. Chem. Phys.* **1995**, 103 (1), 20-36.

13. Bock, C. W.; Trachtman, M.; George, P. *Chem. Phys.* **1985**, 83 (3), 431-443.

14. Frisch, M. J.; Trucks, G. W. Schlegel, H. B. et al. GAUSSIAN 09: Revision C.02 (Pittsburg, PA: Gaussian Inc.) 2009.

15. Frisch, A.; Nielsen, A. B.; Holder, A. J. *Gauss 09 View User Manual (Pittsburg: Gaussian Inc.)* 2009.

16.https://www.acros.com/DesktopModules/Acros_Search_Results/Acros_Search_Results.aspx?search_type=CatalogSearch&SearchString=4-Cyanostyrene (accessed 01.05.2020) .

17. Smith, B. C. *Infrared Spectral Interpretation: A Systematic Approach*; CRC Press, New York, 1998.

18. Rao, J. M. *Organic Spectroscopy Principles and Applications*, Narosa Publishing House, New Delhi, 2000.

19. Kanamori, H.; Endo, Y.; Hirota, E. *J. Chem. Phys.* **1990**, 92 (1), 197-205.

20. Kim, E.; Yamamoto, S. *J. Chem. Phys.* **2002**, 116 (24), 10713-10718.

21. Tanaka, K.; Toshimitsu, M.; Harada, K.; Tanaka, T. *J. Chem. Phys.* **2004**, 120 (8), 3604-3618.

22. Shepherd, R. A.; Doyle, T. J.; Graham, W. R. M. *J. Chem. Phys.* **1988**, 89 (5), 2738-2742.

23. Tanskanen, H.; Khriachtchev, L.; Rasanen, M.; Feldman, V. I.; Sukhov, F. F.; Orlov, A. Y.; Tyurin, D. A. *J. Chem. Phys.* **2005**, 123 (6), 064318.

24. Paolucci, D. M.; Gunkelman, K.; McMahon, M. T.; McHugh, J.; Abrash, S. A. *J. Phys. Chem.* **1995**, 99, 10506-10510.

25. Forney; D.; Jacox, M. E.; Thompson, W. E. *J. Mol. Spectrosc.* **1995**, 170, 178-214.

26. Nikow; M.; Wilhelm, M. J.; Dai, H. L. *J. Phys. Chem. A* **2009**, 113 (31), 8857-8870.

27. Dollish, F. R.; Fateley, W. G.; Bentley, F. F. *Characteristic Raman Frequencies of Organic Compounds*; Wiley: N.Y., USA, 1974.

28. Bellamy, L. J. *The Infrared Spectra of Complex Molecules*; Wiley: N.Y., USA, 1975.

29. Lin-Vien, D.; Colthup; N. B.; Fateley; W. G.; Grasselli; J. G. *The Handbook of Infrared and Raman Characteristics frequencies of Organic Molecules* Academic Press: San Diego, California, 1991.

30. Socrates, G. *Infrared and Raman Characteristic Group Frequencies*, 3rd ed.; Wiley: N.Y., USA, 2004.

31. Krishnakumar, V.; Prabavathi; N. *Spectrochim. Acta A* **2008**, 71 (12), 449-457.

32. Altun, A.; Gölcük, K.; Kumru, M. *J. Mol. Struc-Theochem* **2003**, 637, 155-169.

33. Singh, S. J.; Pandey, S. M. *Indian J. Pure Ap. Phy.* **1974**, 12, 300-304.

34. Lee, S. Y. *B. Korean Chem. Soc.* **1998**, 19 (1), 93-98.

35. Wheeless, C. J.; Zhou, X.; Liu; R. *J. Phys. Chem.* **1995**, 99 (33), 12488-12492.