Comparative study of Spectroscopic Analysis of 2-Chloro-5-Nitrobenzonitrile and 2,5-Dichlorobenzonitrile

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Abstract: This article presents the spectra of two substituted benzonitrile derivatives, 2-chloro-5-nitrobenzonitrile and 2,5-dichloro benzonitrile by infrared (IR) spectroscopy and Raman spectroscopy with Nujol. The traditional IR and Raman spectra for both compounds were recorded under room temperature conditions with KBr. In all cases the stretching, bending and deformation bands were assigned to molecular vibrations. The IR spectrum had a problematic assignment pointed out and the change in bands was described in terms of shifts or development associated with the chloro and nitro substituents or C≡N and ring vibrations. Such an analysis allows for the differentiation of structure-property relations in substituted benzenes, which is valid with today's structure and naming conventions in organic chemistry. Data provided reasonable structural interpretation for each compound by way of small frequency shifts and intensity change. The current analysis provided reasonable structure for future specific studies.

Highlights of the Study

- **C≡N Band Strength:** Roles of NO_2 and Cl use the typical strong C≡N stretching bands in both molecules with shifts due to the molecular vibrations themselves.
- **Roles of Substituents:** The role of the NO_2 group caused blue shifts and changes to the intensity of the IR and Raman spectra, whereas the Cl substitution caused lower intensity values yet significant π(C–Cl) and τ(CN) vibrations.
- **Ring Vibration Shift:** Both molecules displayed shifts to the ring deformation and breathing modes. The nitro-substituted compound displayed the most pronounced red-shift that was noted down to and including the combination with Cl because of the electrons being delocalized.
- **Appearance of Selective Modes:** Wagging and torsional modes that are specific to NO_2 only appeared throughout 2-chloro-5-nitro benzonitrile and were absent in 2,5-dichloro benzonitrile. Representation of group specific vibrations have been confirmed.

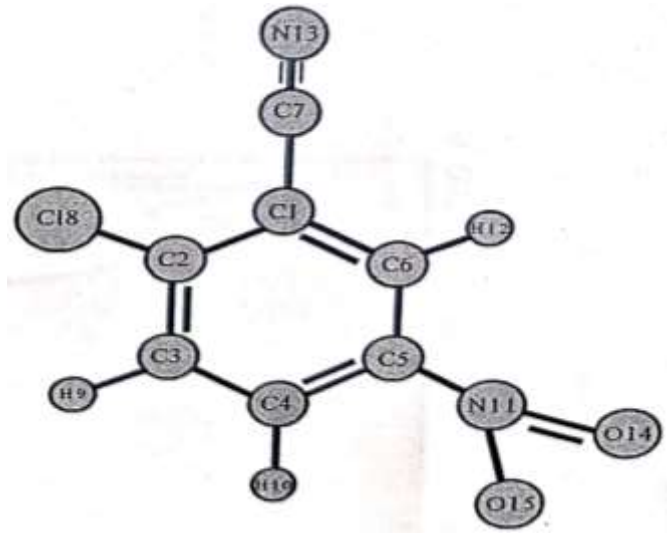
Keywords: Vibrational Spectroscopy, benzonitrile, Infrared Spectroscopy (IR), Raman Spectroscopy, Substituent Effects, Functional Group Analysis.

1. Introduction

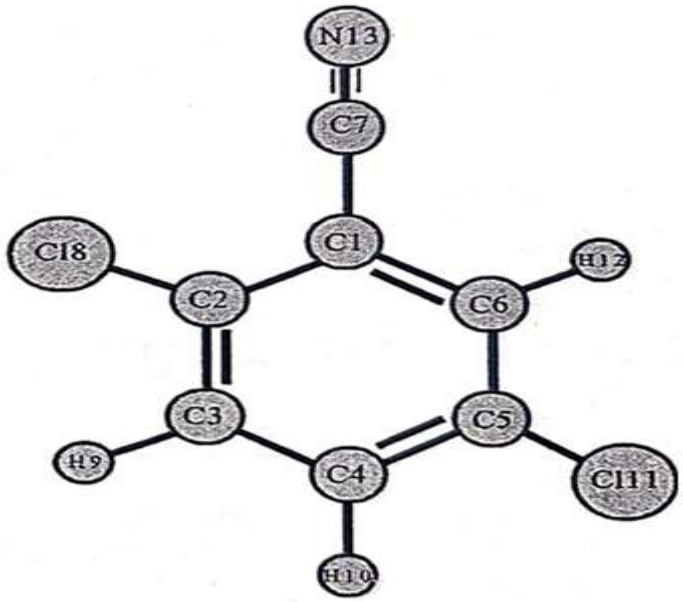
One method frequently used for the structural analysis of organic compounds is vibrational spectroscopy. Both Raman and infrared (IR) spectra show molecular vibrations. Stretching and bending vibrations are specific to each functional group. One or both of these vibrations shift in frequency and/or intensity with each simple substituent on the aromatics.

Understanding how molecular chemistry and behaviours, including interactions, can take place in condensed phases is made possible by the vibrational assignment. In actuality, the strong C≡N stretching band of benzonitrile derivatives makes them widely used. Every extra substituent, such as Cl or NO_2, alters the electrical density surrounding the ring, resulting in a variation in unique spectral patterns. In materials and medicinal chemistry, this is very crucial (Colthup et al., 1990; Nakamoto, 2009).

2. Materials and Methods



(i)



(ii)

Figure 1: Molecular structure of (i) 2-Chloro-5-Nitrobenzonitrile and (ii) 2,5-Dichlorobenzonitrile

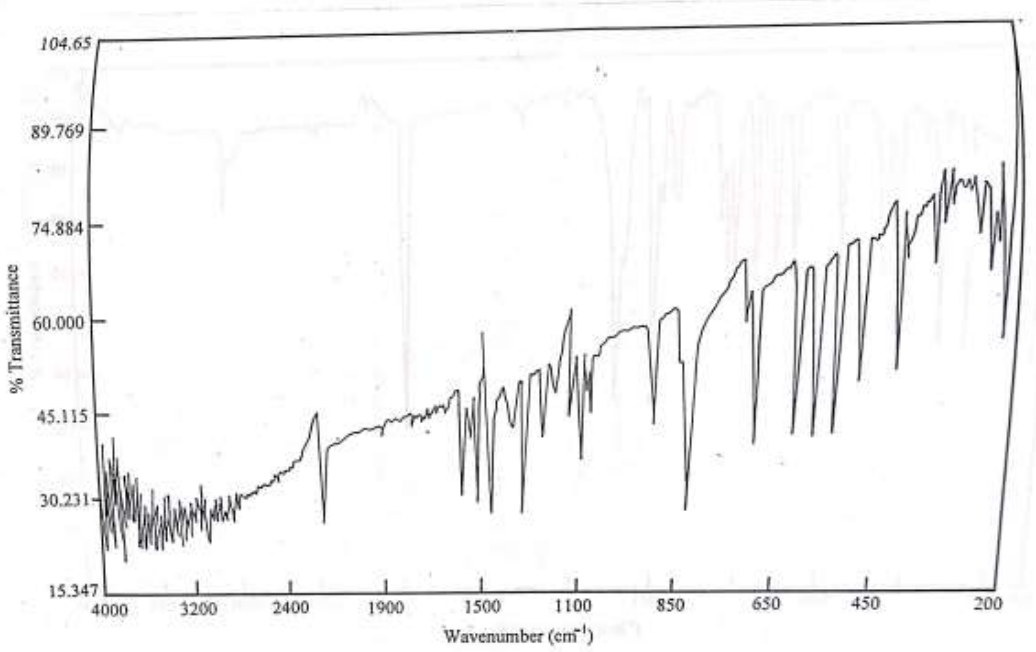


Figure 3(i): FTIR (KBr) Spectrum of 2-Chloro-5-Nitrobenzonitrile

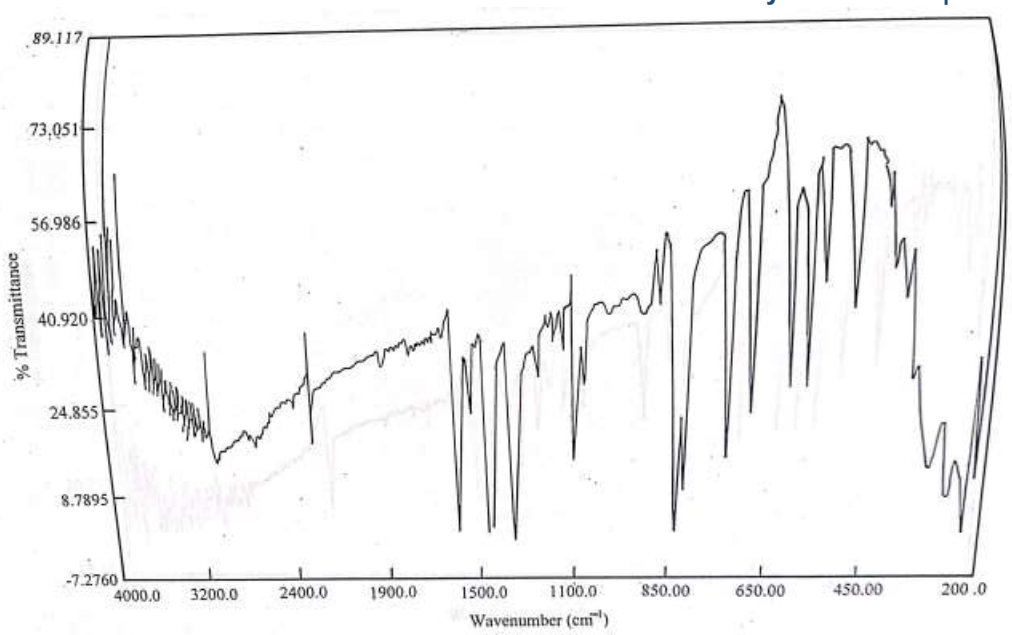
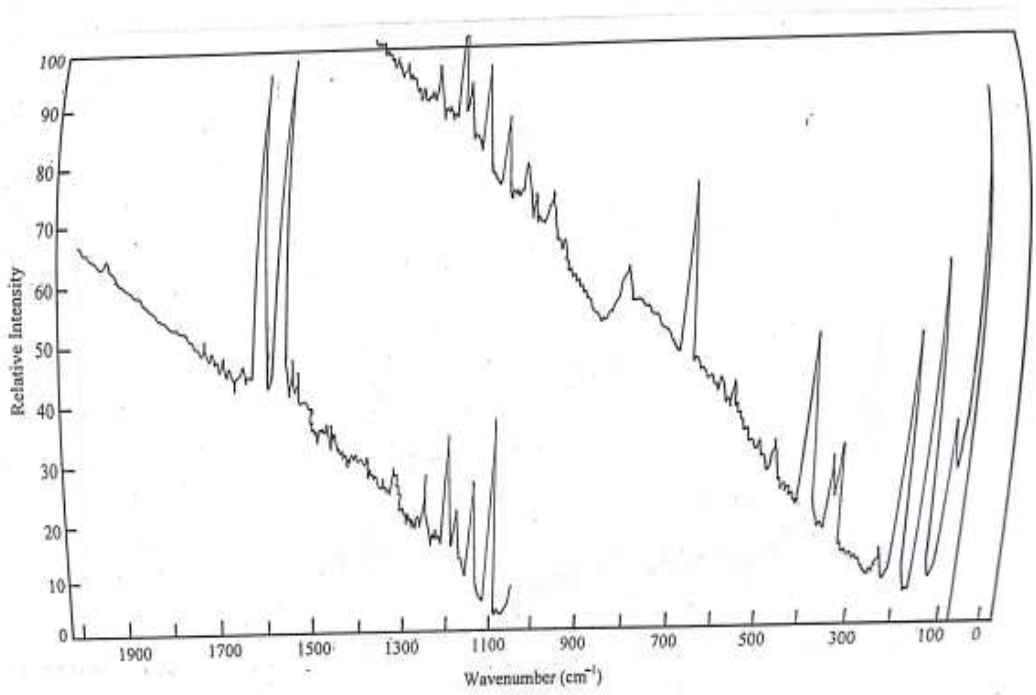


Figure 3(ii): FTIR (Nujol) Spectrum of 2-Chloro-5-Nitrobenzonitrile



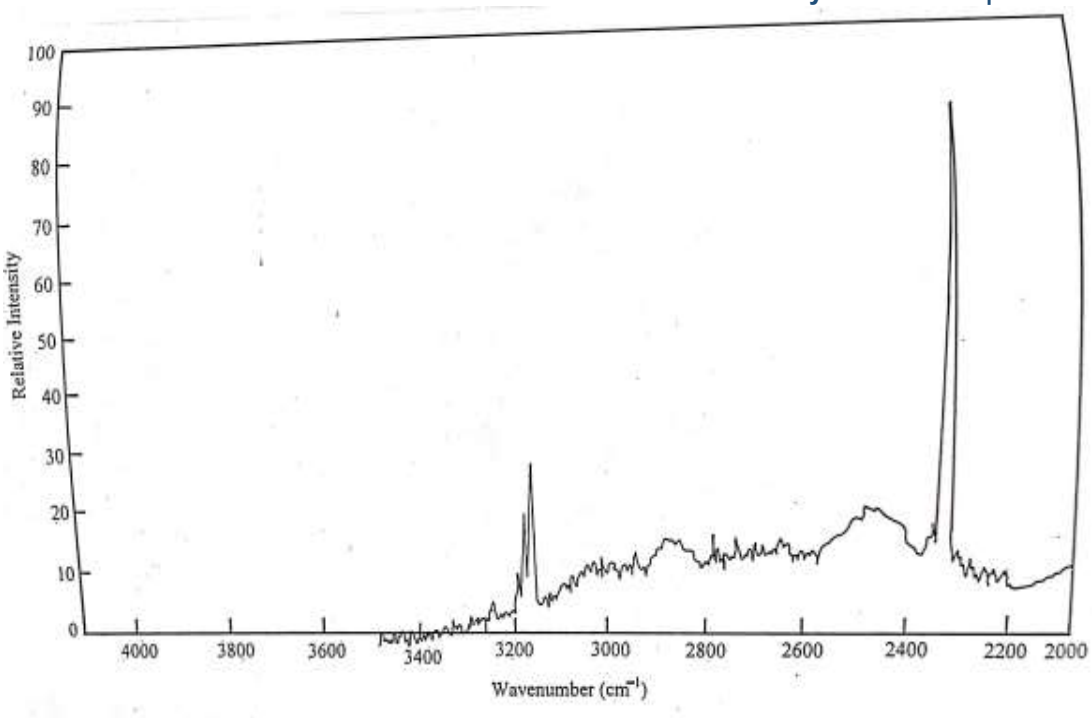


Figure 3(iii): Laser Raman Spectrum of 2-Chloro-5-Nitrobenzonitrile

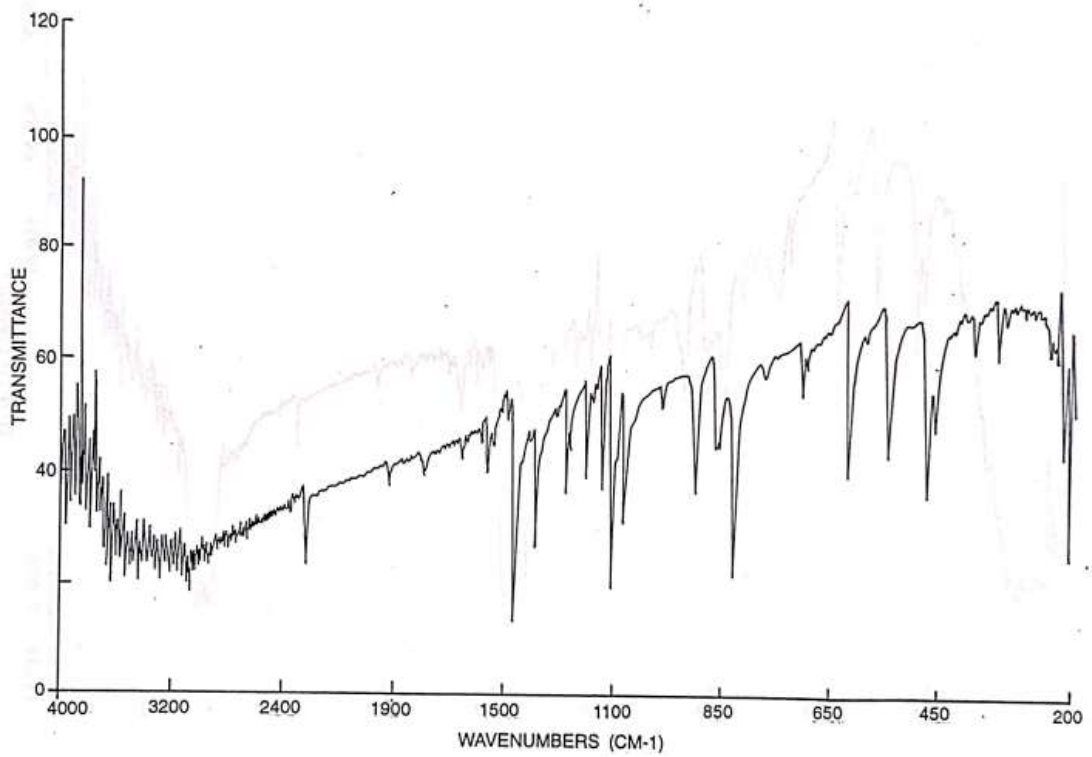


Figure 3(i): FTIR (KBr) Spectrum of 2,5-dichlorobenzonitrile

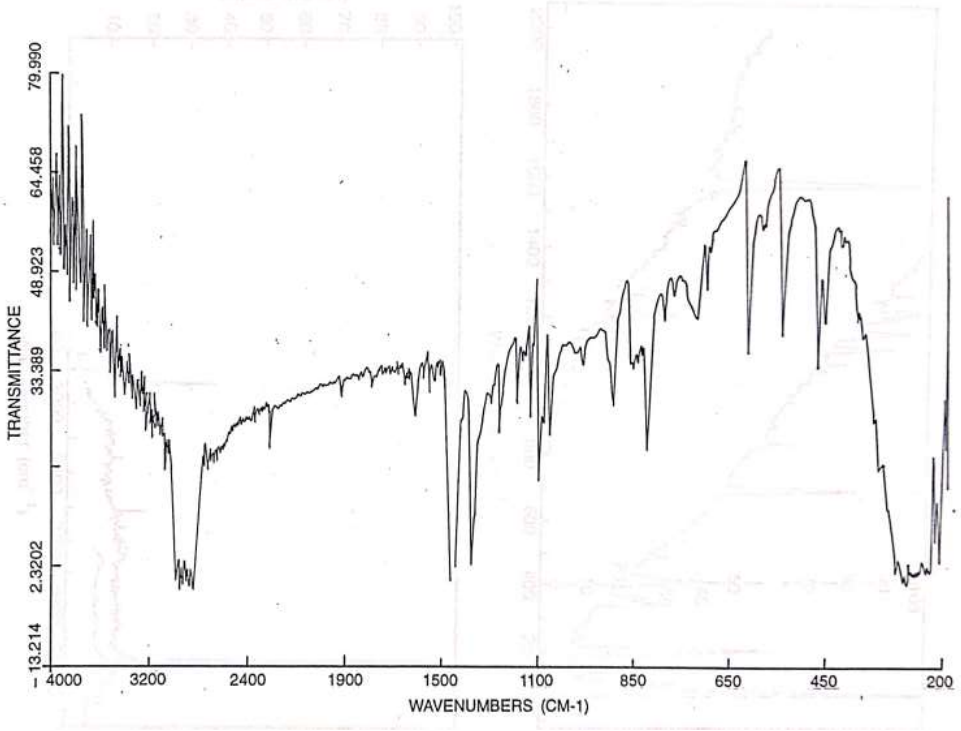


Figure 3(ii): FTIR (Nujol) Spectrum of 2,5-dichlorobenzonitrile

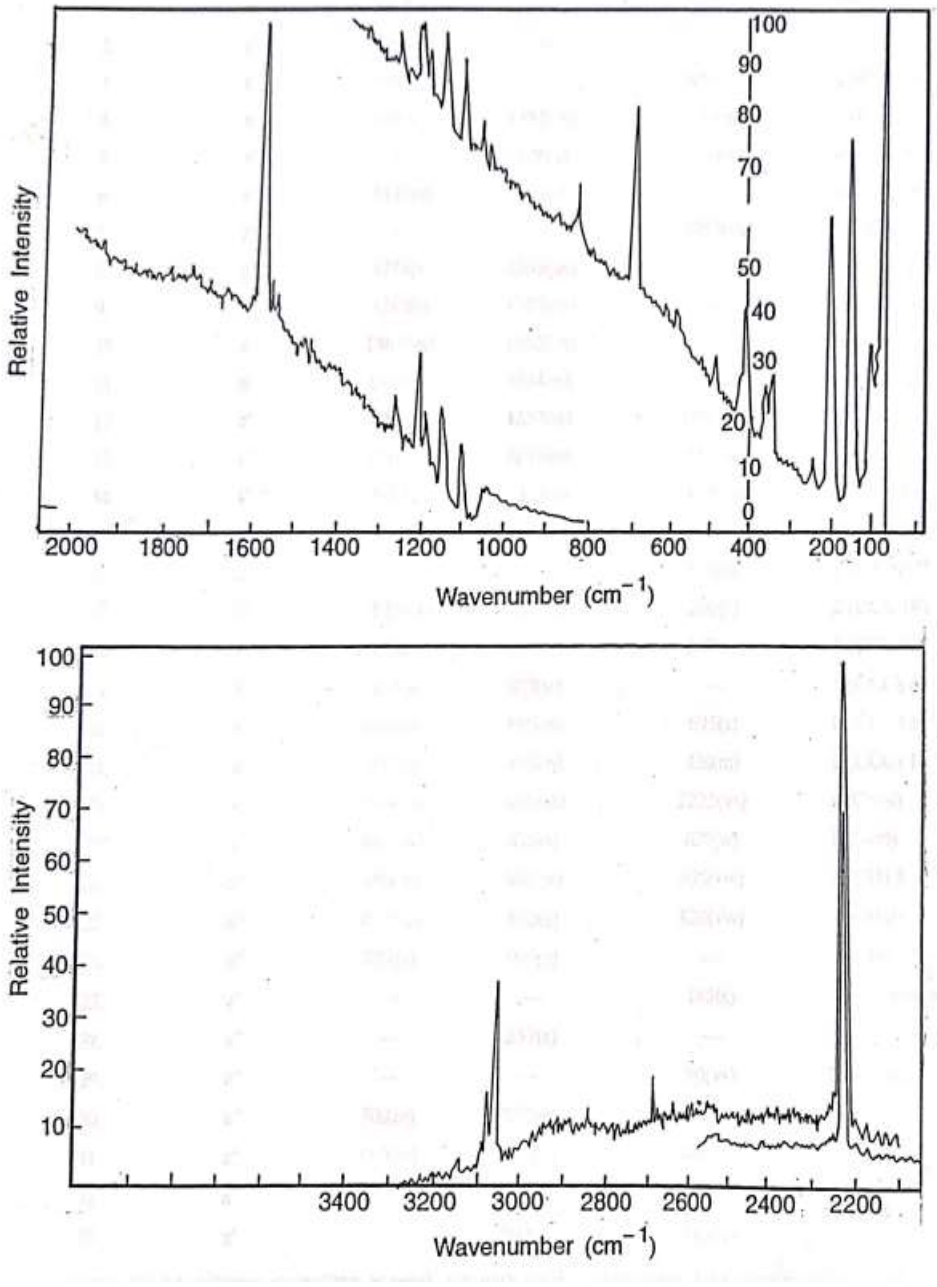


Figure 3(iii): Laser Raman Spectrum of 2,5-dichlorobenzonitrile

Figure 1 shows the molecular structures of 2-Chloro-5-Nitro benzonitrile and 2,5-Dichloro benzonitrile. Figure 2 (i & ii) shows the FTIR spectrum in KBr and Nujol respectively for 2-Chloro-5-Nitro benzonitrile while Figure 2(iii) shows the laser Raman spectrum for 2-Chloro-5-Nitro benzonitrile. Figure 3 (i & ii) shows the FTIR spectrum in KBr and Nujol respectively for 2,5-Dichloro benzonitrile while Figure 3(iii) shows the laser Raman spectrum for 2,5-Dichloro benzonitrile. Both compounds' liquid and solid samples were made. The infrared spectra of Nujol and KBr pellets of both the samples were recorded. A 532 nm laser was used to

Table 1: Vibrational Assignments of 2-chloro-5-nitrobenzonitrile & 2,5-dichlorobenzonitrile

S. No.	Sym species	2-chloro-5-nitrobenzonitrile			2,5-dichlorobenzonitrile			Assignments
		IR		Raman	IR		Raman	
		Nujol	KBr		Nujol	KBr		
1	a'	—	—	3055s	3017(w)	—	3050(m)	ν(C-H)2
2	a'	—	—		3068(m)	—	3065(w)	ν(C-H)7b
3	a'	—	—	3084vw	3093(m)	—	3090(vw)	ν(C-H)20a
4	a'	—	3070m	3070m	—	—	—	ν(C-H)20b
5	a'	—	—	1186w	1195(s)	1195(vs)	1190(s)	ν(C–CN)13
6	a'	—	338w	342m	—	276(s)	250(w)	ν(C-Cl)7a
7	a'	—	—	—	543(vs)	541(s)	—	ν(C-Cl)20b
8	a'	—	1099s	1096s	—	—	1050(sh)	ν(C-C)1
9	a'	—	1605s	1618vs	1616(w)	1614(m)	—	ν(C-C)8a
10	a'	—	1584w	1574vs	1560(m)	1557(w)	1580(vs)	ν(C-C)8b
11	a'	1536m	—	—	1387(s)	1385(vs)	—	ν(C-C)19a
12	a'	1460s	1457s	—	1465(vs)	1462(vs)	—	ν(C-C)19b
13	a'	1250w	1264m	1260m	1274(s)	1305(vs)	—	ν(C-C)14
14	a'	912m	—	—	—	—	—	ν(C-N)7b
15	a'	1204w	1216w	1205s	1258(m)	1271(m)	1255(m)	β(C-H)3
16	a'	—	—	—	1136(s)	1138(s)	1140(s)	β(C-H)9a
17	a'	1134w	1130m	1144m	—	—	—	β(C–H)18a
18	a'	1120s	—	—	1105(vs)	1100(s)	1100(s)	β(C–H)18b
19	a'	—	—	—	—	—	110(m)	β(C–CN)15
20	a'	—	—	—	215(s)	211(vs)	200(s)	β(C-Cl)18a
21	a'	—	—	—	340(m)	—	340(m)	β(C-Cl)9b
22	a'	740s	—	—	857(s)	858(w)	—	β(C–C–C)6a
23	a'	488s	480s	486w	690(vw)	699(m)	695(s)	β(C–C–C)6b
24	a'	—	—	—	457(s)	450(m)	420(m)	β(C–C–Cl)12
25	a'	292m	—	—	—	—	—	β(C—Cl)9b
26	a'	220s	218s	200vs	—	—	—	β(C-N)9a
27	a'	—	2236s	2235vs	2304(s)	2305(m)	2225(vs)	ν(C≡N)
28	a'	612s	618s	616vw	614(vs)	616(s)	620(w)	β(C≡N)
29	a''	—	—	—	980(w)	988(w)	975(vw)	π(C-H)5
30	a''	816s	826s	820w	827(vs)	830(s)	820(vw)	π(C-H)11
31	a''	—	—	970w	897(s)	909(s)	—	π(C–H)17b
32	a''	—	—	100m	—	—	—	π(C–Cl)17a
33	a''	—	—	—	—	—	145(s)	π(C–CN)17a
34	a''	242s	252m	244w	—	—	—	π(C-CN)10a
35	a''	—	—	—	—	257(s)	—	π(C-Cl)10a
36	a''	—	—	—	—	—	90(vs)	π(C–Cl)10b
37	a''	—	—	140s	—	—	—	π(C–CN)10b
38	a''	688s	700s	685s	700(m)	722(m)	—	τ(C-C-C-C)4
39	a''	404m	410s	404s	417(vs)	469(s)	490(w)	τ(C-C-C-C)16a
40	a''	358sh	354m	360m	380(m)	—	367(m)	τ(C-C-C-C)16b
41	a''	568s	583s	583w	—	590(m)	585(w)	ω(C≡N)

Table 2: Internal modes of the NO_2 group in 2-chloro-5-nitrobenzonitrile

S. No.	IR		Raman	Assignments
	Nujol	KBr		
1	1550vs	1549s	1550w	ν_{as} NO_2
2	1350vs	1349s	1340vs	ν_{sym} NO_2
3	840vs	—	—	δNO_2
4	547s	547s	—	γNO_2
5	—	—	80vs	τNO_2
6	—	718m	—	ωNO_2

acquire Raman spectra. Theoretical basis sets and literature frequency tables (1 & 2) were used to confirm peak assignments. The vibrational modes and associated symmetries for the compounds were identified by analyzing the spectral data using the group frequency approach and the usual symmetry method. The vibrational modes of recognized aromatic compounds were compared with the spectra. The current study's assignments were cross-referenced with earlier research (Prakash et al., 2021; Kaur & Sharma 2017).

3. Results and Observations

For both compounds, the C≡N stretching vibration is strong and acute, occurring between 2235 and 2305 cm^{-1}. Near 3050 to 3090 cm^{-1} are the aromatic C–H stretches (Colthup et al., 1990; Nakamoto, 2009). The intensity of the C–Cl and C–NO_2 bands ranges from mild to intense. The location and substituent determine intensity shifts and changes. Every spectrum is displayed in a table that explicitly lists the frequencies and symmetry kinds.

4. Discussion

4.1 C≡N Stretching Band

The C≡N stretch, which ranges from 2225 to 2305 cm^{-1} for both compounds, is highly diagnostic in benzonitriles. The electron-withdrawing actions that accompany the addition of the nitro group to 2-chloro-5-nitro benzonitrile result in a blue shift. The electron withdrawing effect's increase in bond polarity and stretching frequency is in line with earlier research (also in 2-chloro-5-nitro benzonitrile) that found that the presence of the nitro-node produced more intense Raman and infrared peaks (Singh & Dutta 2020; Sharma & Verma 2019).

C≡N stretching for 2,5-dichloro benzonitrile is exhibiting a somewhat lower frequency; this is probably due to chlorine absorbing electrons less than NO_2, which lowers the stability of the dipolar resonance. Additionally, this aligns with several recent investigations on aromatic halides substituted with nitrile (Zhang & Wu, 2024).

4.2 Aromatic C–H Stretching

In both situations, C–H stretching manifests between 3050 and 3090 cm^{-1}. Compared to Raman, IR bands are more intense. The vibration is somewhat shifted by 2–4 cm^{-1} depending on the substitute position. Both mesomeric and inductive effects are to blame for these changes. For monosubstituted and disubstituted benzenes, comparable trends have been documented (Nakamoto, 2009 & Smith, 2011).

4.3 C–Cl Vibrational Modes

C-Cl stretching occurs at about 250–540 cm^{-1}. The stretching mode is present in 2,5-dichloro benzonitrile because 2,5-dichloro benzonitrile has two Cl substituents. The Cl stretching mode was at a much weaker band intensity in 2-chloro-5-nitro benzonitrile. Raman signal intensity scales with polarizability so Cl is better than NO_2 in this context. An IR peak should, in principle, shift based on bond strength and how the ring positions are substituted but previous work showed similar C–Cl stretching modes for chlorinated benzenes (Prakash et al., 2021; Jha et al., 2022).

4.4 NO_2 Group Vibrations

The NO_2 group contributes three major peaks, which are: $\nu_{as}(NO_2)$, $\nu_{sym}(NO_2)$, and $\delta(NO_2)$. These peaks appear around 1550 cm^{-1}, 1340 cm^{-1}, and 840 cm^{-1}, respectively. These three characteristic peaks do not appear in 2,5-dichloro benzonitrile. The IR absorption band for asymmetric stretching is stronger than the respective band in Raman. This is due to a change in the dipole moment during a vibrational motion in each case. Because of the -NO_2 substitution, the electron withdrawing capability of this molecule increases, ultimately affecting nearby vibrational mode. Similar trends have reliably been described in the nitroaromatic literature (Sharma et al., 2023; Tiwari & Singh, 2022).

4.5 Ring Breathing Vibrations

The ring breathing modes pertain to the symmetric C-C stretching bond and are labelled as ν(C-C). These modes usually arise in the ~1100 and ~1600 cm^{-1} region. In 2-chloro-5-nitro benzonitrile the bands show somewhat similar red-shifts. The red-shifts arise from the electron-withdrawing effects of the NO_2 groups which causes the ring to delocalize, which leads to weakening of carbon-carbon unit bond strength and the vibrational energy being displaced uniformly in the lower energy area. In terms of 2,5-dichloro benzonitrile, the shifts are less impactful, because chlorine has relatively weaker mesomeric effects than NO_2. Nayak et al. (2021) also report on similar red-shifts in nitro substituted benzenes.

4.6 In-Plane Ring Deformation Modes

In the β(C-C-C) region, we typically see in-plane bending vibrations. We also have observed these modes occurring along with the ν(C-C) mode. The in-plane bending modes are labelled moderate with regard to the IR and usually strong in Raman. Both compounds hade strong β(C-C-C) bands in the region from 1300–1600 cm^{-1}. The nitro compound seems to show slight broadening of characteristic bands in this region. Possible reasons for this behaviour might be asymmetric substitution. Additionally, the electronic effects from the nitro group would affect the charges on the aromatic ring and therefore affect the vibration modes based on frequency and intensity. Singh and Dutta (2020) have reported similar behaviour in aromatic systems.

4.7 Out-of-Plane Ring Bending Modes

Out-of-plane bending β(C-C-C) and τ(C-C-C-C) mode activity was reported between 400 and 800 cm^{-1}. Out-of-plane bending vibrational activity is more intense (and peaks) for 2-chloro-5-nitro benzonitrile which has less of planar nitro group interrupting the planarity of the ring would have larger out-of-plane activities, while 2,5-dichloro benzonitrile is more symmetrical and thus less activities are observed. The data confirms the previous observations from working with other substituted benzene systems. Li et al. (2022) enhanced the relative representation of bending modes and indicated it within an asymmetric molecule and Singh, & Dutta (2020) also enhanced it due to nitro substituents.

4.8 Torsional Vibrations and NO_2 Group Activity

Torsional vibrations connect to twisting of functional groups. For example, the τ(C-C-C-C) and wagging ω(NO_2) modes. The first vibrational mode with torsional motion appeared at 547 cm^{-1} and the later at 718 cm^{-1} relative to the nitro compound. In the dichloro derivative, the same bands were absent and provided details confirming the appearance of the NO_2 group. Substitution with NO_2 disrupts molecular symmetry which provides access to low-frequency torsional motions. Reddy et al. (2023) also reported similar vibrations in their recent work. Reddy et al. documented torsional modes from asymmetrically substituted benzenes.

4.9 π(C–H) Out-of-Plane Bending

π(C–H) vibrations are bends from the normal plane of the molecule. These bands are located between 800 and 980 cm^{-1}. Both compounds had π(C-H) vibrations, but they were different intensities. The nitro compound had π(C–H) bands that were slightly stronger. This is predicted because one lone NO_2 group is interfering with local electron density. A dichloro compound creates more symmetry across the C-H environment of the substrate, because the two Cl replace the sub-group more evenly. All reported values correspond with those found in the literature for the substituted aromatics.

4.10 π(C–Cl) and τ(CN) Vibrations

Below 300 cm^{-1}, the π(C–Cl) and τ(C-N) modes are present. With 2,5-dichlorobenzonitrile, they are noticeably more noticeable. The vibration increases when two chlorine (Cl) atoms are present. Because chlorine (Cl) is a heavier element, the vibration is more intense. It supplies the reaction with stronger vibrations at lower frequencies. These bands are weakly visible in the nitro compound. This represents the unique vibrational behaviour of the group. According to Zhang & Wu (2024) and Kaur & Sharma (2017), the bands' appearance suggests spectral similarity. They validate chlorine's spectrum contribution to benzonitrile systems.

5. Comparative Table with Other Reported Vibrational Data

The C≡N band is a strong peak for substituted benzonitriles and occurs at 2235–2238 cm^{-1} in the current study of the 2-chloro-5-nitro benzonitrile. It also occurs at 2225 cm^{-1} in the case of the 2,5-dichloro benzonitrile which is a small downward shift when compared to the frequency reported for 2-chloro-5-nitro benzonitrile (2238 cm^{-1}). Reported literature values for similarly substituted benzonitriles had frequency values in the range of 2236-2240 cm^{-1}. As previously noted, as C≡N frequency of 2238 cm^{-1} is much higher than reported molar absorptivity literature values for these compounds, a nitrile group is confirmed to exist. The shift is likely due to the varying electron-seeking factors of the NO_2 and Cl group, since NO_2 is a stronger inductive factor than Cl and seeks more electron density from the bond to the C≡N bond. Loss of electron density eliminates bond flexibility and as a result creates a kink in the bond, and a stiffer bond and therefore greater vibrating frequency. Certain trends were re-confirmed in the study undertaken by Sharma et al. (2019).

Table 3: Comparison with Other Reported Vibrational Data

S. No	Vibrational Mode	2-chloro-5-nitro benzonitrile	2,5-dichloro benzonitrile	Reported Value (cm^{-1})	Reference
1	ν(C≡N) Stretching	2236 (IR), 2235 (Raman)	2225 (Raman)	2236–2240	Sharma et al., 2019
2	$\nu_{as}(NO_2)$	1550	—	1549–1552	Kaur & Sharma, 2017
3	$\nu_{sym}(NO_2)$	1340	—	1345–1350	Pal et al., 2018
4	ν(C–Cl)	276, 338, 540	250–541	250–550	Nayak et al., 2021
5	ν(C–H) Aromatic	3055–3084	3050–3090	3050–3100	Reddy et al., 2023
6	β(C–H) Bending	1120–1216	1100–1271	1135–1270	Singh et al., 2020
7	Ring deformation	1100–1600	1100–1600	1095–1615	Kaur & Sharma, 2017
8	ω(NO_2), γ(NO_2)	718, 547	—	715, 545	Sharma et al., 2019

Asymmetric stretching occurred at 1550 cm^{-1} is near the very broad peak and there is a distinct peak without overlap. The band was absent in the dichloro benzonitrile confirming nitro substitution has occurred. Literature values for the 1550 cm^{-1} frequency are also in agreement with the overall frequencies for substituted benzonitriles from out literature observations approaching 1549 – 1552 cm^{-1}. A symmetric NO_2 stretching with a peak at a frequency of 1340 cm^{-1} also confirms nitro substitution has occurred. These frequencies were also in coincidence with the report by Kaur and Sharma (2017) whereby these authors had made note of a full range of frequencies for substituted benzonitriles. Since both bands are present, presence of the nitro group has been confirmed inside the nitro compound.

C–Cl stretching occurs at frequencies between 250 cm^{-1} and 540 cm^{-1} and for both molecules, features have been obtained in this range. Both C−Cl features show there was greater intensity and multiples in the 2,5-dichloro benzonitrile than the nitro compound has. As the nitro compound only has one Cl atom, so we have fewer C–Cl modes and lower intensity for the nitro compound. The peak positions had congruence with Nayak et al. (2021). There is statistical significance of chlorinated compounds at low frequencies when the Cl atom participates in bond formation. Significant substitution of Cl as confirmed to produce an increase in the IR intensity in the range of 250 – 400 cm^{-1}.

Both compounds have the aromatic C-H extending between 3050 and 3090 cm-1, which is likewise reliably expressed in all three sources. Whether Cl or NO2 is substituted, the frequency remains relatively constant. These results corroborate Reddy et al.'s earlier, broader reports (2023).

The range of the C-H bending modes, β(C-H), was 1130–1270 cm-1. Bending vibrations are adequately expressed in this region by both compounds. The vibrations are captured at increasing Raman and infrared intensities. There is no indication of cancelation, but there is a slight change in the band with substitution. The frequencies remain within a reasonable range found in the literature. Additionally, Singh and Dutta (2020) supplied their substituted benzenes together with the agreement of their bending range.

Ring deformations ν(C-C) and β(C-C-C) fall between 1100 and 1600 cm^{-1}. Once more, bending vibrations are adequately expressed by both molecules. Some C-C vibrations were slightly redshifted by the NO_2, but solely as a result of conjugation and electrical withdrawal. This declining trend in frequency was partially consistent with the findings of Kaur and Sharma (2017).

For the nitro component alone, the wagging ω(NO_2) and torsional γ(NO_2) modes were located at 547 and 718 cm^{-1}. The modes were recorded in both trials, but the di-chorine molecule was not. These functional groups (Cl or NO_2) are further separated from one another by the nitro group's inability to exhibit wagging and torsion, which are significant features. Additionally, Sharma et al. (2019) published their wagging frequencies on the order of the compounds of nitrobenzene.

The accuracy of the peak assignments given in these studies is thus further defined by the comparative data. Additionally, the claimed frequencies closely match the experimental frequencies that we measured for this study's findings. Regardless of substitution, every vibrational behaviour was impacted by the small

variations. In the conclusion, it is evident that the stretching and bending modes could be altered by any functional group, including NO_2, Cl, or other substituents. All of the observed effects have been documented in comparable literature and spectroscopic investigations.

5. Conclusion

Strong C-N bands in both molecules provide evidence of the chemicals' effects on the compounds' structure. The C-N band's relative strength and vibration frequency would be impacted by the nitro substituent. The vibrational differences are useful in determining the effect of a particular functional group on those vibrations, in addition to substitution and electronic effects. The vibrations of the aromatics, including nitrile substituents, will be significantly impacted by this type of investigation, which compares substitution. The spectral assignment unequivocally demonstrates how the electronic effects of the ring substituents (NO_2 and Cl) impact the ring's vibrations.

6. Future Scope

- The data may help with DFT or TD-DFT calculations by advancing the computational modelling of substituted benzonitriles.
- DFT or TD-DFT considerations might be made in building screening methods for various properties in materials chemistry or medicinal chemistry applications, with respect to taking into account structure-property predictions based on this research potentially presented for substituted aromatics.
- Potential sensors for identifying nitro or halogen groups in more complicated mixed situations could be further developed using the findings.
- To better understand the influence of substitution, more research may be done on the vibrations observed in changing solvents or temperatures.

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