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NOTES

Laser Raman and Infrared Spectra of 4-Amino-2-Chlorobenzonitrile

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Laser Raman and infrared spectrum of 4-amino-2-chlorobenzonitrile have been recorded in solid phase. The spectrum has been analysed assuming C_s point group for the molecule and the observed fundamentals have been assigned to different normal modes of vibration.

We have been investigating the vibrational features of substituted benzonitriles with a view to investigate the effect of different substituents at different positions.[1,2] In the present study, the vibrational spectrum (IR and Raman) of 4-amino-2-chlorobenzonitrile has been investigated.

The IR in CsI (200–4000 cm^{-1}) and laser Raman spectra (100–2400 cm^{-1}) of this compound have been recorded and the observed fundamental bands have been assigned on the basis of group frequency approach (Table 1). The molecule has been considered as belonging to

TABLE 1

ASSIGNMENTS OF VIBRATIONAL FREQUENCIES (in cm^{-1}) OF 4-AMINO-BENZONITRILE AND 4-AMINO-2-CHLORO-BENZONITRILE

4-aminobenzonitrile		4-amino-2-chloro-benzonitrile			Assignments
IR	Raman	sym	IR	Raman	
—	—	a′	3460 m	—	NH_2 asym. stretch
3340 s	—	a′	3367 s	—	NH_2 sym. stretch
—	—	—	3238 s	—	N–H stretch
3205 s	—	—	3218 s	—	N–H stretch
—	—	a′	3120 vw	—	νC–H
—	—	a′	3070 w	—	νC–H
3048 w	—	a′	3045 s	—	νC–H
2197 vs	2210 vvs	a′	2236 vs	2232 s	νC≡N

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TABLE (cont.)

4-aminobenzonitrile		4-amino-2-chloro-benzonitrile			Assignments
IR	Raman	sym	IR	Raman	
—	1628 w	a′	1634 s	—	NH_2 scissor
1595 vs	1599 vs	a′	1592 m	1604 m	νC–C
1516 m	1520 w	a′	1510 m	1515 w	νC–C
1500 m	—	a′	1496 sh	—	νC–C
—	—	a′	1388 vs	—	νC–C
—	1340 w	a′	1338 m	1332 vw	νC–NH_2
1319 vvs	1314 vw	a′	1316 vs	1314 vw	νC–C
1217 m	1220 m	a′	1215 m	1220 m	βC–H
—	1196 w	a′	1202 sh	1200 vw	βC–H
1177 vs	1173 vs	a′	1175 vs	1170 s	νC–CN
1140 s	1138 w	a′	1136 s	—	βC–H
—	—	a″	—	1075 w	NH_2 twisting
1012 m	—	a′	1008 w	—	φC–C–C
970 m	976 vw	a″	960 m	—	νC–H
948 m	—	a″	943 w	935 w	νC–H
832 vs	842 s	a″	835 vs	846 vs	νC–H
—	819 sh	a′	827 s	820 w	νC–C (ring breath)
742 w	—	a″	—	—	νC–H
717 w	702 w	a″	715 s	720 m	δC–C–C
682 vs	—	a′	680 s	—	NH_2 wagging
—	—	a′	670 s	675 s	νC–Cl
535 vs	—	a′	538 vs	534 w	βC≡N
475 vw	490 vw	a′	470 vw	480 w	φC–C–C
—	420 w	a″	410 vs	—	δC–C–C
372 sh	389 vw	a′	380 s	393 w	βC–NH_2
330 vs	—	a′	336 m	—	βC–CN
250 sh	265 vw	a″	246 sh	245 vw	νC≡N
—	240 sh	a″	233 sh	—	νC–NH_2
230 sh	—	a″	224 s	—	νC–CN
—	—	a″	215 s	—	NH_2 torsion
—	—	a″	200 vs	—	νC–Cl

the point group C_s, with the assumption that the substituents are coplanar with the benzene ring. This simplified model leads to 30 normal vibrations for the phenyl ring, of which 21 are planar (a′) and 9 non-planar (a″). In addition to these, there will also appear group vibrations due to –CN and –NH_2 groups.

4-Amino-2-chlorobenzonitrile may be derived theoretically from 4-aminobenzonitrile by the replacement of H at C_2 position by a Cl atom. In order to see the effect of substituent at C_2 position (Cl in the present case) on the internal vibrations of -CN and NH_2 groups, the assignment of vibrational spectrum of 4-aminobenzonitrile in the same phase has also been included in Table 1.

The CN stretching vibrations has been strongly observed both in the IR (2236 cm^{-1}) and Ramanspectrum (2232 cm^{-1}). The $C\equiv N$ in-plane-bending vibration has been identified at 538 cm^{-1} in IR and at 534 cm^{-1} in Raman; and $C\equiv N$ out-of-plane bending vibration at 246 cm^{-1} in IR and at 245 cm^{-1} in Raman spectrum in the present case. The strong IR bands observed at 3460 and 3367 cm^{-1} have been assigned to the N–H (NH_2) assymmetric and symmetric stretching vibrations respectively. The bands observed at 3238 and 3218 cm^{-1} correspond to NH_2 bonded stretching vibrations. The C-Cl stretching vibration has been identified as the strong band at 670 cm^{-1} in IR and at 675 cm^{-1} in Raman spectrum. These assignments are in agreement with the data available for related molecules[2–7]. The assignment of other vibration of the compound studied are presented in Table 1.

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