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Vibrational Analysis of Phenyl Butazone

V. KRISHANAKUMAR, N. SUNDARESAN† and A. NATARAJAN*
Department of Physics, Nehru Memorial College,
Puthanampatti, Tiruchirapalli, India.

The laser Raman spectrum of phenyl butazone was recorded in the region 4000–200 cm^{-1} and its fourier transform infrared spectrum in the region 4000–400 cm^{-1}. The spectra have been analysed assuming C_1 point group symmetry. Probable assignments to the observed bands have been made with the help of magnitude and intensities of the recorded spectra.

INTRODUCTION

Phenyl butazone is considered for the present study because of its biological, pharmaceutical and analgesic character. The probable structure of the molecule is shown in Fig. 1. The Molecule under investigation is a non-planar molecule with C_1 symmetry. Phenyl butazone being a 43 atomic molecule, would give rise to 123 normal modes of vibrations. Detailed band assignments of all the modes

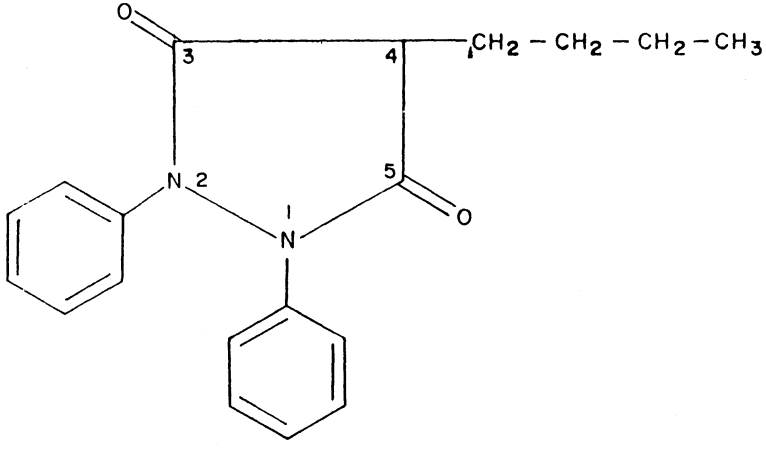

Fig. 1

†Department of Physics, National College, Tiruchirapalli-620 001, India.
*Department of Physics, Bharathidasan University, Tiruchirapalli-620 024, India.

are not possible for this type of molecules, because of their high complexity and low symmetry.

EXPERIMENTAL

Pure solid sample of phenyl butazone was obtained from the Department of Chemistry, Nehru Memorial College. The F.T.I.R. spectra was recorded in KBr disc on Perkin-Elmer F.T.I.R. spectrometer in the region 4000-400 cm^{-1}. The laser Raman spectrum was recorded in the standard 90° configuration in the region 4000-200 cm^{-1} on Dilor Z-24 Raman spectrometer. Argon ion laser operating at 200 MW power continously on the 488 nm line was used as the laser source.

RESULTS AND DISCUSSION

The observed infrared and Raman frequencies of Phenyl butazone, together with relative intensities and assignments are given in Table-1.

O—H Stretching: The two bands occuring at 3647 cm^{-1} and 3607 cm^{-1} in 2-tert-butyl phenol were assigned to O—H stretching modes by the earlier workers[1-5]. Moreover the broad wings of the O—H stretch can be seen on either side of the narrow C—H bands. Consideration of these factors lead to assign the weak absorption bands at 3849 cm^{-1}, 3425 cm^{-1} in IR and 3750 cm^{-1}, 3468 cm^{-1} in Raman to O—H stretching vibrations. The large band width of the O—H band could be due to inter/intramolecular association.

C—H Stretching: Infrared absorption bands due to the C—H stretching modes of organic compounds[6] occur in the region of 3000 cm^{-1}. Hence, the bands observed at 3058 cm^{-1}, 2925 cm^{-1} and 2870 cm^{-1} in IR and 3069 cm^{-1}, 2926 cm^{-1} and 2863 cm^{-1} in Raman spectra have been designated as the C—H stretching modes.

C=O Stretching: According to Bellamy[6] the absorption band at 1716 cm^{-1} for a five membered ring ketone is due to C=O stretching. Therefore, the two strong bands observed at 1751 cm^{-1} and 1717 cm^{-1} have been assigned to C=O stretching vibrations.

C=C Stretching: The bands at 1630 cm^{-1} in IR and 1627 cm^{-1} in Raman spectra were assigned to C=C stretching modes for isomeric methyl styrenes by the earlier workers.[7] In the present study, the bands observed at 1655 cm^{-1}, 1618 cm^{-1} and 1594 cm^{-1} in IR and the bands at 1671 cm^{-1}, 1604 cm^{-1} and 1501 cm^{-1} in Raman spectra have been assigned to C=C stretching modes of vibration.

CH_3 Group Vibrations: The assignments made by the earlier workers[8-10] in CH_3 group vibrations lead to assign the following bands to the various modes.

The symmetric and asymmetric deformation modes of CH_3 group of phenyl butazone are assigned to 1325 cm^{-1}, 1495 cm^{-1} in IR and 1353 cm^{-1}, 1443 cm^{-1} in Raman spectra. From the observation of bands it appears that the frequency shift between symmetric and asymmetric modes are 170 cm^{-1} in IR and 90 cm^{-1} in Raman spectra.

The weak band observed at 1153 cm^{-1} is assigned to CH_3 rocking mode. The bands at 1101 cm^{-1} in IR and 1013 cm^{-1} in Raman spectra are assigned to CH_3

stretching modes of vibration. The low frequency region at 504 cm^{-1} in IR and 502 cm^{-1} in Raman spectra are designated as CH_3 torsional mode.

TABLE-1
ASSIGNMENTS OF FUNDAMENTAL FREQUENCIES OF PHENYL BUTAZONE

F.T.I.R. observed frequencies (cm^{-1}) and intensities	Laser Raman observed frequencies (cm^{-1}) and intensities	Assignments
3849 w	3750 w	O—H Stretching
3425 w	3468 w	O—H Stretching
3058 m	3069 m	C—H Stretching asymmetric
2925 m	2926 m	C—H Stretching asymmetric
1751 s	—	C=O Stretching
1717 s	—	C=O Stretching
1655 s	1671 m	C=C Stretching
1618 w	1604 vs	C=C Stretching
1594 m	1501 w	C=C Stretching
1495 ms	1443 w	CH_3 deformation asymmetric
1455 m	—	CH_2 deformation
1413 w	—	C—H deformation
1325 w	1353 m	CH_3 deformation symmetric
1295 m	—	C—H in-plane deformation
1195 s	—	C—N Stretching
1175 w	1165 w	CH_2 Wagging
1153 w	—	CH_3 Rocking
1101 w	1013 vs	CH_3 Stretching
1026 w	—	CH_2 Twisting
900 w	—	O—H deformation out-of-plane
864 w	—	C—H Wagging
810 vw	—	C—H deformation
753 s	—	CH_2 Rocking
696 s	681 s	out-of-plane deformation
642 w	—	C=O out-of-plane deformation
597 m	605 s	Planar ring beding
560 w	—	C = O in-plane deformation
523 w	—	Ring deformation
504 w	502 m	CH_3 Torsion
464 w	—	Skeletal mode
—	265 w	Phenyl group vibrations

vs—very strong, s—strong, m—medium, ms—medium strong, w—weak, vw—very weak.

CH_2 Group Vibrations: The bands at 1455 cm^{-1}, 1026 cm^{-1} and 753 cm^{-1} in IR are assigned to CH_2 deformation, twisting and rocking modes respectively. These assignments, are supported by the earlier literature values[10, 11]. The weak bands observed at 1175 cm^{-1} in IR and 1165 cm^{-1} Raman spectra are assigned to CH_2 wagging mode.

In-Plane and Out-of-Plane Vibrations: The band at 1295 cm^{-1} is assigned to C—H in-plane deformation. This assignments is in close agreement with the literature values.[11] The weak band at 560 cm^{-1} is designated as C = O in plane deformation mode. The strong bands identified at 696 cm^{-1} in IR and 681 cm^{-1} in Raman spectra are assigned to C = O out of-plane deformation.

Earlier workers[12] defined the vibrations at lower frequency regions as due to phenyl group. Hence, in the present study the band at 265 cm^{-1} in Raman is assigned to phenyl group vibrations.

Conclusion

It is concluded that conincidence between IR and Raman bands in the spectra, rules out the possiblity of the molecule possessing centre of symmetry. Moreover, the observed spectra reveals the complementary nature of the IR and Raman spectra.

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