



Vibrational Spectroscopy

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Vibrational assignments of infrared and laser raman spectra of nitrofurazone

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ABSTRACT

Over several years, 5-Nitro 2-Furaldehyde Semicarbozone, otherwise known as Nitrofurazone has been in widespread use as anti-bacterial drug. The recording of FTIR and Laser Raman Spectra is done for the characteristic vibrations of C=N, N-N and furan ring systems and the tentative vibrational assignments have been reported. In the present investigation, vibrational assignments has been carried out for the molecule of the title compound using fundamental modes of vibration observed in Infrared and Raman Spectroscopy. The vibrational modes are classified into a' and a'' irreducible representations. Thus 42 fundamental modes of vibration ie.29a' and 13a'' vibrations are considered. A satisfactory vibrational band assignment has been made by using the FTIR Laser Raman Spectra of the compound.

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Introduction

Nitrofurazone is a centrally acting anti-bacterial drug. But the mechanism of anti-bacterial action of the furan derivatives is still unknown. But the presence of nitro group in the 5th position may be responsible for anti-bacterial activity on many 2-substituted furans. So the recording of two spectra is done for the characteristics vibrations of C=N, N-N and furan ring systems and the tentative vibrational assignments have been reported. In the present investigation, the vibrational assignments are supported by group frequency table.

Experimental

The fine sample of Nitrofurazone is got from Eskay Laboratory Ltd. Bangalore, and it was used as in such without any further purification. The sample is soluble in dimethyl fluoride and slightly soluble in water, but it is insoluble in ether and chloroform. The infrared spectrum of Nitrofurazone was recorded in the region 4000-200 cm⁻¹ using nujol on Perkin Elmer model 599 of spectro photometer. The laser Raman spectrum of the above compound was recorded in the region 4100-100cm⁻¹, on a spex spectrometer using 5145 Å lines of spectra physics organ-ion laser at 300mw of power. The frequencies for all sharp bands are accurate to ±cm⁻¹. The infrared laser Raman spectra of Nitrofurazone are shown in fig's 2,3 and 4 respectively.

Molecular structure and symmetry

The molecular structure of Nitrofurazone is shown in fig.1 by assuming NO₂ and NH as point masses the molecule under investigation is assumed to have C point group symmetry. The vibrational modes are classified at transforming like the basis functions of and an irreducible representation. Thus the 42 fundamental modes of vibrations of Nitrofurazone may be classified into 29 a symmetry species (in plane) and 13 a species (out of plane) vibrations.

Results and discussion

The observed and calculated frequencies of Nitrofurazone along with assignments are shown in table 1, 2 and 3. The vibrational assignments of all the in-plane and out-plane modes of vibrations are made by referring to the assignments of the corresponding bands in related systems, intensities of the

spectrum and potential energy distributions. The vibrational assignments are discussed in the following.

N-H vibrations: The Nitrofurazone which is under investigation has NH₂ group and hence asymmetric and symmetric NH stretch vibrations are possible. The NH stretching frequency of aromatic compounds occurs in the region 3300-3500 cm⁻¹ are assigned to NH₂ asymmetric AND symmetric group of vibrations. The bands at 3460 cm⁻¹ and 3380 cm⁻¹ are due to N-H stretching modes of vibrations appear in group are found to be stronger when compared to N-H ring vibrations.

C-H vibrations: The characteristic region of C-H stretching vibrations are around 3000-3100 cm⁻¹. The weak infrared bands of Nitrofurazone identified at 3310, 3260, 3140 and 2940 cm⁻¹ have been designated to C-H stretching modes of vibrations.

C-N vibrations: The medium band observed at 2850 cm⁻¹ in 5 methyl cytosine has been assigned to C=N aliphatic symmetry stretching. This leads to assign the weak bands at 2880 cm⁻¹ to C=N aliphatic symmetry stretching modes of vibrations. The infrared bands at 1510, 1475, 1470, 1355 and 1340 cm⁻¹ are due to C-N stretching vibrations. The band width between single and double bond regions are found to be satisfactory. The corresponding Raman bands for this mode are 1470 and 1350 cm⁻¹.

C=O Stretching: In general the characteristic C=O stretching vibrations of cyclic ketones are found in the region 1800-1000 cm⁻¹ depending on the ring size. The C=O frequencies increase with ring strain. The title compound shows bands at 1820 and 1780 cm⁻¹ respectively. The increase in frequency has established strain on the ring and the intensity of the carbonial band is essentially the same in all compounds. The stretching vibrations of single bonded carbon and oxygen atoms have been noticed at 1255 and 1220 cm⁻¹.

C-C Vibrations: The C-C stretch vibrations occur nearly at 1600cm⁻¹. In the present study the bands due to C-C stretching vibrations are appearing at 1590 and 1580 cm⁻¹ respectively. The bands are not much affected due to nature of the substitutes in this region. The peak observed at 1710 cm⁻¹ is due to C=C stretching vibrations.

NH₂ Vibrations. The rocking and twisting modes of amino group of Nitrofurazone have been observed at 1160 and 1128 cm⁻¹. The NH₂ out of plane bending vibrations has been identified at 502 cm⁻¹. The carbonyl out of plane bending vibration occurs at 417 cm⁻¹. The out of plane bending vibration due to the ring of Nitrofurazone appears at 590 cm⁻¹ both in Infrared and Raman.

In plane vibrations: The CH in plane bending vibrations of the title compound has been identified at 1330, 1320, 1310 and 1260 cm⁻¹ respectively. The weak infra red bands at 1020 cm⁻¹ and Raman bands 1018 and 970 cm⁻¹ have been fixed at C-N in plane bending vibrations. The weak band at 1080 cm⁻¹ in infrared is due to CCC trigonal bending vibrations.

Out of plane vibrations: The three weak bands identified at 952, 930 and 905 cm⁻¹ is due to C-H out of plane bending vibrations. The weak and medium infrared bands at 840 and 816 cm⁻¹ and the medium, strong Raman bands at 810 cm⁻¹ have been identified to NH out of plane bending vibrations. The C-C out of plane vibrations occur at 775 cm⁻¹. The carbons trigonal out of plane bending vibrations are identified at 790, 756 and 376 cm⁻¹. The bands at 740 and 660 cm⁻¹ in infrared and weak Raman band 600 cm⁻¹ have been assigned to C-N out of plane bending.

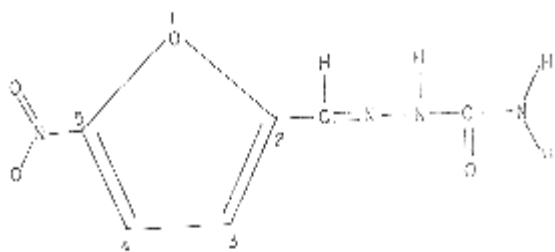


Fig.1

Conclusion

Thus a complete vibrational band assignment of Nitrofurazone has been carried out using infrared and laser Raman spectra on the basis of cs point group symmetry. A systematic set of symmetry co-ordinates has been constructed and the vibrational assignments have been calculated.

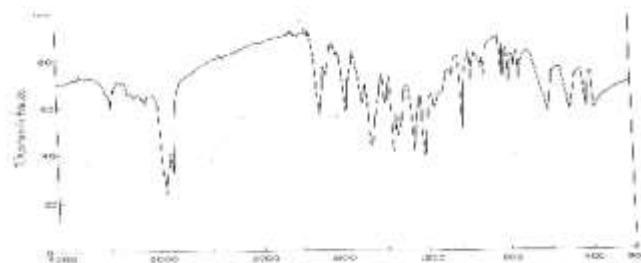


Fig.2

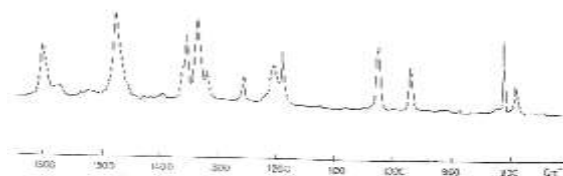


Fig.3

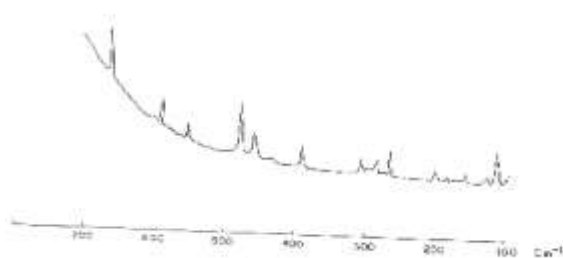


Fig.4

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Table 1. Vibrational assignments of nitrofurazone

Species	Infrared frequencies cm ⁻¹	Relative strength	Laser Raman frequencies cm ⁻¹	Relative strength	Calculated frequencies cm ⁻¹	Assignments
a'	3520	W	-	-	3512	NH2 asymmetric stretching
a'	3480	W	-	-	3462	NH2 asymmetric stretching
a'	3460	S	-	-	3354	N-H stretching
a'	3380	VW	-	-	3371	N-H stretching
a'	3310	VW	-	-	3301	C-H stretching
a'	3260	VW	-	-	3250	C-H stretching
a'	3140	VW	-	-	3134	C-H stretching
a'	2940	M	-	-	2935	C-H stretching
a'	2880	M	-	-	2870	C=N aliphatic symmetric stretching
a'	2840	VW	-	-	2334	C=N aliphatic symmetric stretching
a'	1820	VW	-	-	1811	C=O stretching
a'	1780	S	-	-	1776	C=O stretching
a'	1710	W	-	-	1693	C=O stretching
a'	1590	W	1595	s	1594	C-C stretching
a'	1580	M	-	-	1571	C-C stretching
a'	1510	M	-	-	1496	C-N stretching
a'	1475	M	-	-	1478	C-N stretching
a'	1470	VS	1470	vs	1462	C-N stretching
a'	1355	S	1350	ms	1351	C-N stretching
a'	1340	BR	1340	ms	1349	C-N stretching
a'	1330	S	-	-	1321	C-H in plane berndong
a'	1320	W	1320	-	1324	C-H in plane berndong
a'	1310	S	-	-	1314	C-H in plane berndong
a'	1260	W	-	w	1266	N-N stretching
a'	1255	S	1250	sh	1251	C-O stretching
a'	1220	S	-	-	1212	C-O stretching
a'	1206	W	1206	w	1196	C-H in plane berndong
a'	1160	W	1190	m	1151	NH2 rocking
a'	1128	M	-	-	1124	NH2 twisting
a'	1080	W	-	-	1076	CCC trigonal bending
a'	1020	W	1018	s	1011	C-N in plane bending
a'	1008	S	-	-	1006	CCC in plane bending
a'	980	W	970	m	971	C-N in plane bending
a''	952	W	-	-	958	C-H out of plane bending
a''	930	W	-	-	921	C-H out of plane bending
a''	905	W	-	-	891	C-H out of plane bending
a''	840	W	-	-	849	N-H out of plane bending
a''	816	M	810	ms	812	N-H out of plane bending
a''	790	W	-	-	789	CCC out of plane bending
a''	775	M	775	w	768	CCC out of plane bending
a''	756	M	-	-	736	CCC out of plane bending
a''	740	M	-	-	712	C-N out of plane bending
a''	660	M	660	w	654	C-N out of plane bending
a''	590	W	590	w	587	Ring out of plane bending
a''	502	W	-	-	511	NH2 out of plane bending
a''	417	VW	-	-	421	C=O out of plane bending
a''	376	VW	385	-	360	CCC out of plane bending