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# FTIR SPECTRUM OF 1-BROMO-3-FLUORO-4-IODOBENZENE

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## ABSTRACT

The present study deals with the infrared absorption spectrum of 1-bromo-3-fluoro-4-iodobenzene. The infrared absorption spectrum of 1-bromo-3-fluoro-4-iodobenzene has been recorded on Perkin Elmer spectrophotometer in the region 400-4000 $cm^{-1}$ using KBr pellet technique. The analysis of spectrum has been made and the assignment of fundamental frequencies to various modes of vibration have been proposed by using these frequencies.

**Key words:** FTIR spectra, 1-bromo-3-fluoro-4-iodobenzene.

## INTRODUCTION

Some of the vibrational modes of benzene are substituent sensitive. To understand this, the vibrational study of substituted benzenes is desirable. Literature is available on mono and disubstituted benzenes[1,2]. However on trisubstituted benzenes such studies are limited. The assignment of vibrational frequencies of some trisubstituted benzene compounds was made by Deb and Banerjee[3] by studying the Raman and infrared spectra of the compounds. Such assignment was not made by any previous worker in the case of 1-bromo-3-fluoro-4-iodobenzene. In fact the infrared spectra of 1-bromo-3-fluoro-4-iodobenzene was not known. The present investigation was undertaken to study the infrared spectra of said molecule.

## EXPERIMENTAL

The compound 1-bromo-3-fluoro-4-iodobenzene of spectroscopic grade was obtained from sigma-Aldrich chemical co. U.S.A. and used as such. The infrared spectrum was recorded on perkin Elmer spectrophotometer in the region 400-4000 $cm^{-1}$ by using KBr. Pellet technique.

## RESULTS AND DISCUSSION

The structural diagram of 1-bromo-3-fluoro-4-iodobenzene is given in fig. 1. Infrared absorption spectra of molecule under investigation is shown in fig.2. Aromatic compound shows the C-H stretching absorption in the region 3000-3100 $cm^{-1}$ [4]. In said molecule there are two C-H stretching frequencies at 3022 and 3073 $cm^{-1}$ in the infrared

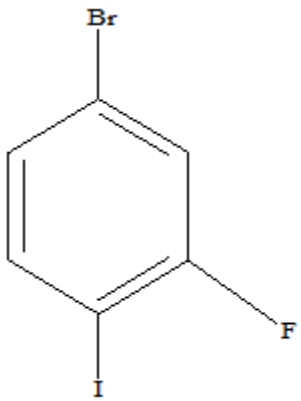


**Fig. - 1: 1-bromo-3-fluro-4- iodobenzene**

spectrum. Whiffen[5] has been able to show that all the bands assigned with reasonably high precision to summation bands of the C-H out of plane fundamental which occur between 700-1000 $cm^{-1}$ [6]. In the infrared spectrum, there are usually a number of medium to weak sharp bands in the region 1000-1300 $cm^{-1}$ region many of which involve in plane C-H bending vibration[7]. Some times strongly mixed with C=C vibration[8,9]. The same result have been observed in the spectrum of the compound (Table - 1).

The appearance of a group of six bands in the region 1000-1650 $cm^{-1}$ represent C=C stretching modes. All the frequencies are known to remain practically unaffected by substitution. These modes in the title compound are in agreement with the literature available for substituted benzenes[10]. In substituted benzene the strong C-F stretching vibrations are appear near 1220 $cm^{-1}$ and 1250 $cm^{-1}$ [10, 11]. One C-Br stretching vibrational frequency has been assigned at 568 $cm^{-1}$ and C-I Stretching vibration frequency has been assigned at 1275 $cm^{-1}$ [11].

**Table - 1: Observed vibrational frequencies of FTIR spectrum of 1-bromo-3-fluoro-4-iodobenzene**

| Frequencies ($cm^{-1}$) | Intensity | Assignments |
|---|---|---|
| 445 | vs | C=C in Plane Bending |
| 500 | s | C=C out of Plane Bending |
| 535 | s | C=C out of Plane Bending |
| 568 | vs | C-Br stretching |
| 684 | w | C-H out of plane bending |
| 701 | vw | C-H out of plane bending |
| 807 | s | C-H out of plane bending |
| 858 | s | C-H out of plane bending |
| 934 | w | C-H out of plane bending |
| 1031 | vs | C-H in plane bending |
| 1077 | vs | C-H in plane bending |
| 1100 | m | C-H in plane bending |
| 1134 | m | C-H in plane bending |
| 1220 | s | C-F stretching |
| 1250 | m | C-F stretching |
| 1275 | m | C-I stretching |
| 1393 | s | C=C stretching |
| 1433 | w | C=C stretching |
| 1500 | w | C=C stretching |
| 1556 | ms | C=C stretching |
| 1572 | w | C=I stretching |
| 1617 | w | C=I stretching |
| 1877 | w | - |
| 2317 | w | - |
| 2709 | w | - |
| 3022 | w | C-H stretching |
| 3073 | mw | C-H stretching |

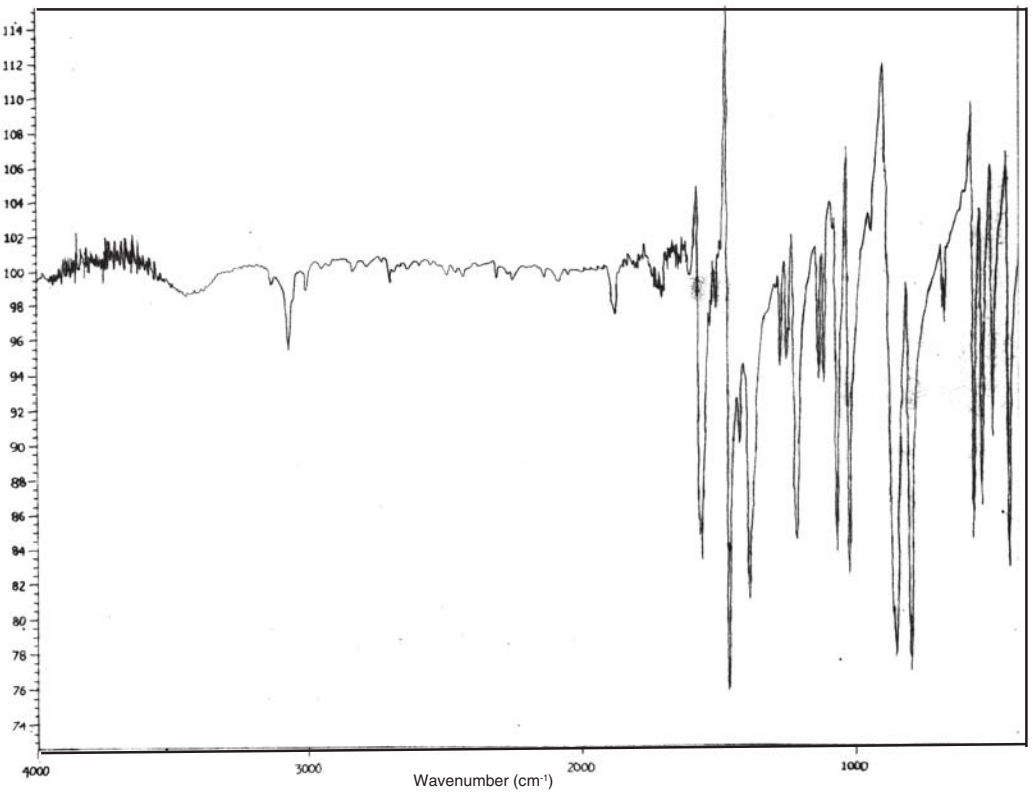


**Fig. - 2: I.R. Spectra of 1-Bromo - 3-fluoro - 4-iodobenzene in KBr pellets**

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**REFERENCES**

1. Yadav R. A., Ph.D. Thesis (Banaras Hindu University, Varanasi), India (1983).
2. Shanker R., Ph.D. Thesis (Banaras Hindu University, Varanasi), India (1991).
3. Deb K. R., and Banerjee S.B., I*nd J. Phys.,* **34,** 554 (1960).
4. Rao C.N.R., Chemical applications of Infrared Spectroscopy, Academic Press, New York, London (1963).
5. Whiffen, *Spectrochim. Acta,* **7,** 253 (1955).
6. Bellamy L. J., The Infrared Spectra of Complex Molecules, Chapman and Hall London (1975).
7. Katrizky A.R., *Quart. Rev. Chem. Soc.,* **13,** 353 (1959).
8. Scherer J.R., *Spectrochim. Acta*., **21,** 321 (1965).
9. Colthup, Daly, Wiberley, Introduction to Infrared and Raman Spectroscopy, Academic Press, New York, San Fransisco, London (1975).

10. Aralakkanavar M.K., Katti N.R., Rekho Rao, Jeergal P.R., Shashidhar M.A., *Indian, J. Pure app. Phys.,* **29,** 569-572 (1991).

11. Shukla J.V. Upadhy K.N. Rai D.K., *Ind. J. Phys.,* **48,** 53-57 (1974).