International Journal of Chemical Science
www.chemicaljournals.com
Online ISSN: 2523-2843
Received: 24-11-2025, Accepted: 19-01-2026, Published: 03-02-2026
Volume 10, Issue 1, 2026, Page No. 34-37

Chemical composition of aromatic halogenated derivatives determined by IR spectroscopy

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Abstract
In this article, we determined the chemical composition of the following halogenated aromatic derivatives: chlorobenzene, iodobenzene and bromobenzene using the Bruker IFS spectrophotometer for wavelengths between 4000 and 100cm^{-1}. These halogenated aromatic derivatives have the following functional groups: C-H, C-C, C-Cl, C-Br, C-I.

Keywords: Chemical composition, IR spectroscopy, aromatic derivatives

Introduction

The high reactivity of halogenated compounds explains their importance for organic synthesis, being very important reaction intermediates. There are halogenated compounds used as alkylating agents, with applications in cancer chemotherapy [1, 5].

Some of the small-molecule halogenated compounds are used as solvents in synthesis laboratories, analysis and in industry: chloroform, methylene chloride, trichloroethene, etc. Some halogenated compounds are important for the polymer industry. For example, vinyl chloride is used to obtain polyvinyl chloride, a polymer with very good mechanical and chemical resistance, 2-chlorobutadiene is used to obtain artificial rubber, tetrafluorene is used for Teflon, etc.

Freons, mixed chlorinated and fluorinated compounds of methane, are used as propellants for substances packaged in aerosol form and as refrigerants.

Some high-molecular polyhalogenated compounds are used as lubricants or insulating agents (decachlorobiphenyl) [6, 12].

There are halogenated compounds used as pesticides (insecticides, herbicides, fungicides). The use of halogenated compounds, especially pesticides, raises environmental pollution problems due to their high stability, which determines their accumulation and persistence in environmental factors, plant and animal organisms, and freons have negative effects by destroying the ozone layer.

Materials and methods

The FT-IR spectrum of the clorbenzene, brombenzene and iodbenzene was recorded in Bruker IFS 66 V spectrometer in the range of 4000 to 100 cm^{-1}.

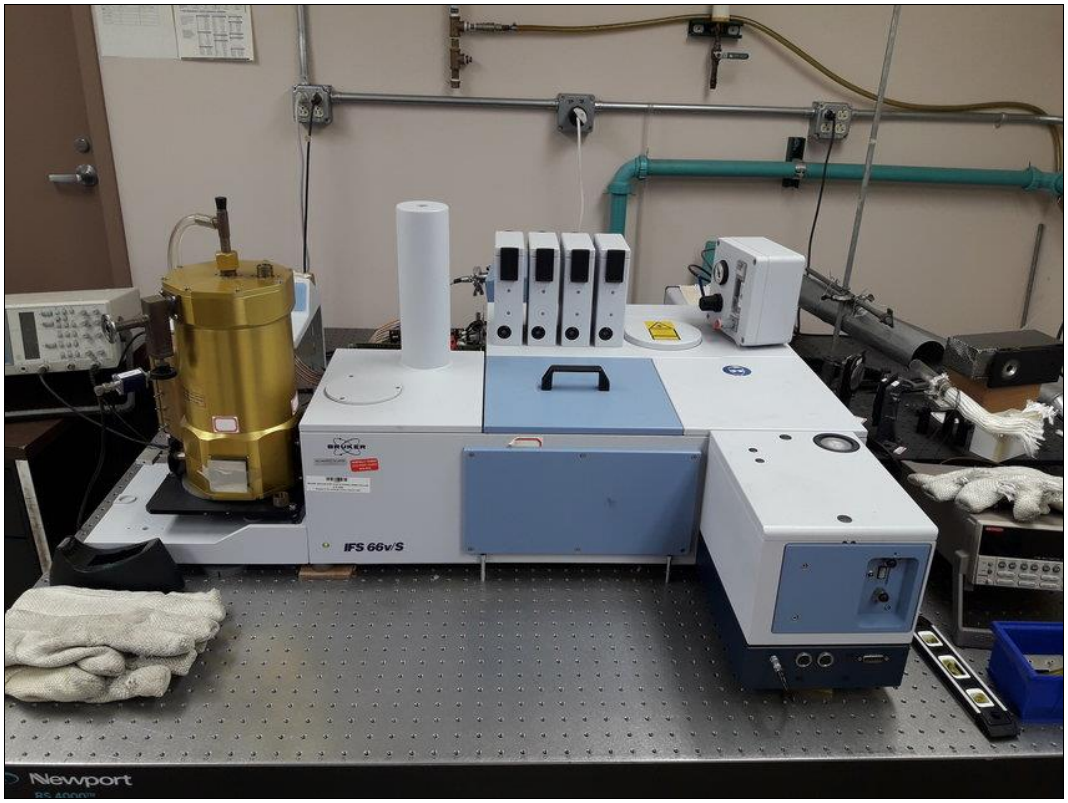

Fig 1: Bruker IFS 66 V spectrometer

Results and discussions

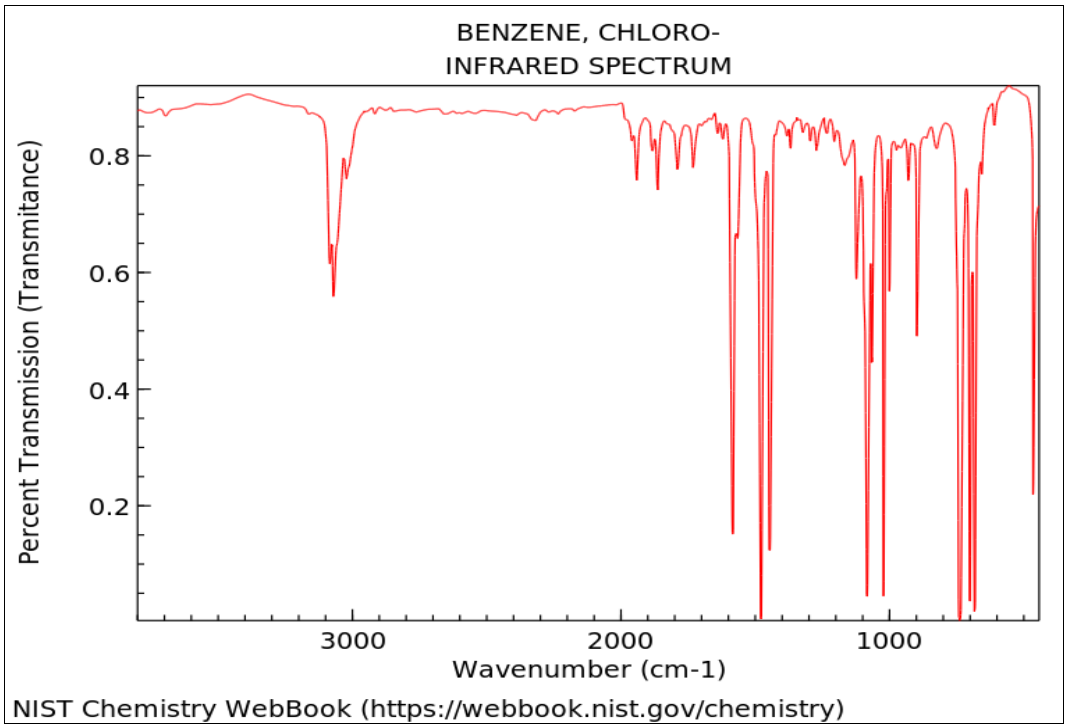

Fig 2: Spectrul IR al clorbenzenului

The most prominent infrared absorption lines of chlorobenzene C-H stretching vibrations of the benzene ring, wavenumbers 3080 to 3030 cm-1.

Several bands of strong absorptions with peaks at wavenumbers ~1500 and 1600 cm^{-1} from C $\cong C$ stretching vibrations of the benzene ring (NOT C=C as in alkenes).

Between wavenumbers 880 and 550 cm-1 are several overlapping absorption bands from C-H and C-Cl vibrations.

The absence of other specific functional group bands will show that particular functional group is absent from the chlorobenzene molecular structure (fig.2) [13, 17].

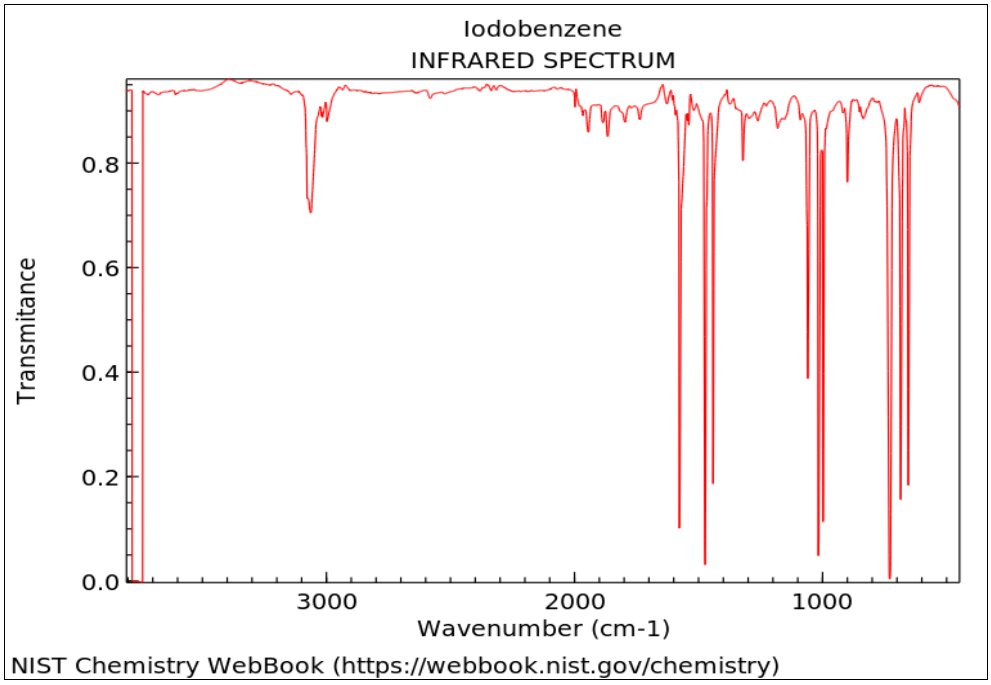

Fig 3: Spectrul IR al iodbenzenului

Spectrul Ir al iod benzenului este cuprins intre lungimile de unda 3031 si 681cm^{-1} (fig. 3).

Tabelul 1 prezinta numarul de unda, gruparea functionala si modul de vibrare pentru iodbenzenul studiat prin spectroscopie IR.

Table 1: Assignments of the vibrational spectra of iodbenzene(C_6H_5I)

Numărul de undă, cm^{-1}	Gruparea funcțională	Modul de vibrare
3031	C-H	stretching
1577	C-C	stretching
1468	C-C	stretching
1175	CCH	In plane bend
1060	C-I	stretching
997	Ring Breathing	-
835	C-H	out- of -plane bend
904	C-H	out- of -plane bend
729	C-H	out- of -plane bend
681	CCC	Nonplanar twist
1435	CC	stretching
1321	CC	stretching
1259	*CCH*	In plane bend

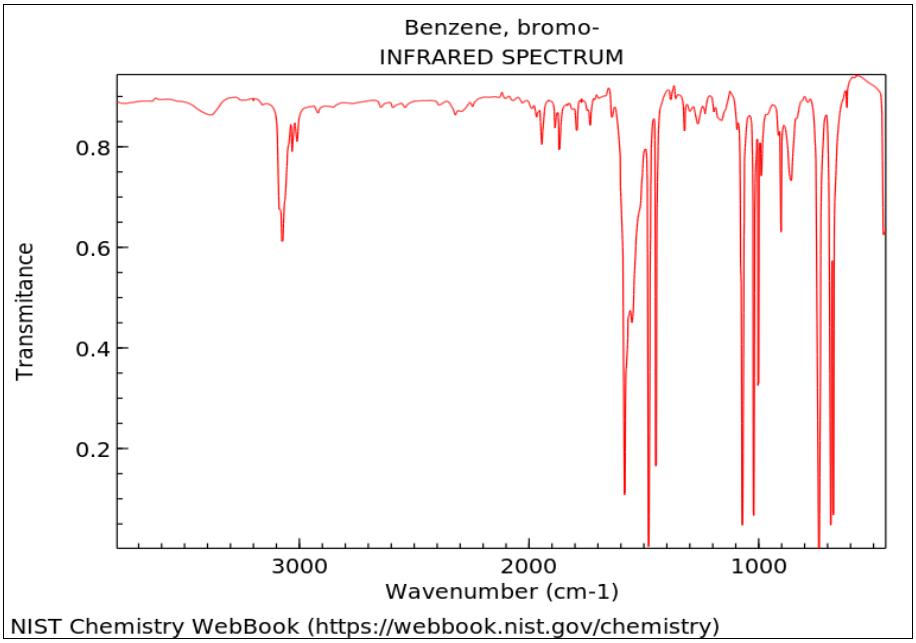

Fig 4: Spectrul IR al brombenzenului

Spectrul IR al brom benzenului este cuprins intre lungimile de unda 4000 si 500cm^{-1}. This vibration is associated with C-H stretching 3400 cm^{-1}. This vibration is associated with C-C stretching in the ring 1700cm^{-1}. This vibration is associated with C-H oscillations 1469 cm^{-1}.This vibration is associated with C-Br stretching 1185 cm^{-1}.This vibration is associated with C-H wag 1007 cm^{-1}. This vibration is associated with C-Br stretching 727cm^{-1}. This vibration is associated with C-C stretching in the ring 681 cm^{-1} (fig.4).

Conclusions

Some of the small-molecule halogenated compounds are used as solvents in synthesis laboratories, analysis and industry: chloroform, methylene chloride, trichloroethene, etc. Some halogenated compounds are important for the polymer industry.

These aromatic halogenated derivatives have the following functional groups in their composition: C-H, C-C, C-Cl, C-Br, C-I.

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