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Study of the composition of phthalic esters by IR spectroscopy

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Abstract
In this article, we determined the composition of phthalic esters by IR spectroscopy using a Jasco 430 FT-IR spectrophotometer. Before determining the composition of the phthalic esters, we synthesized them in a single step. The synthesized phthalic esters are: isodecyl 2-phenoxy ethyl phthalate, isotridecyl 2-phenoxy ethyl phthalate, and isodecyl 2–(o-sec-butyl-phenoxy) ethyl phthalate. These phthalic esters have the following functional groups in their composition: CH_3, C=O, Ar-C-CH_2.

Keywords: Composition, ester, phthalates, spectrum

Introduction

Phthalic esters, also known as phthalates, are derivatives of phthalic acid, characterized by the presence of an aromatic nucleus and two ester groups –COO–. The general structure is that of phthalic acid diesters, in which the hydroxyl groups of the acid are esterified with monovalent alcohols. The general formula can be expressed as follows:

$C_6H_4(COOR)_2$,

where R represents the alcohol radical originating from the alcohol used in the esterification reaction [1, 5].

Changes in the length and structure of the R radicals determine a wide range of compounds with different physicochemical properties. For example: short radicals (methyl, ethyl) → more volatile esters; long or branched radicals → more stable and less water-soluble plasticizers.

Phthalic esters have several common characteristics: oily liquids or viscous solids, depending on molecular weight; low solubility in water, but miscible with organic solvents (alcohols, ketones, chlorinated hydrocarbons); high boiling points and low vapor pressure (at large radicals); relatively good thermal stability, which recommends them as plasticizers.

The exact properties depend on the nature of the alcohol radical, influencing the behavior of the esters in polymers and industrial applications.

Phthalic esters are commonly prepared by the esterification reaction of phthalic acid or phthalic anhydride with the corresponding alcohols, in the presence of an acid catalyst.

Common catalysts include mineral acids (H_2SO_4), organic acids or solid acids (zeolites). The reaction is favored by the continuous removal of the water formed.

Classification is made according to the alcohol radical

- **Short-chain phthalates:** DMP (dimethyl phthalate), DEP (diethyl phthalate), which are more volatile.
- **Medium-chain phthalates:** DBP (dibutyl phthalate), DIBP.
- **Long-chain phthalates:** DEHP (di-2-ethylhexyl phthalate), DINP, DIDP – used mainly as plasticizers for PVC [6, 12].

This diversity allows the plasticizer properties to be adapted to specific applications.

Phthalic esters are used in many areas, in particular: as plasticizers** for PVC (cables, toys, flexible plastics), in adhesives, varnishes, paints and sealants, in cosmetics (certain types with low molecular weight).

Long-chain phthalates are the most widely used due to their stability and good compatibility with polymers.

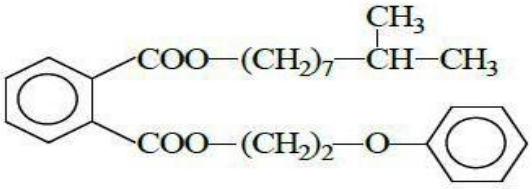
Certain phthalates (especially DBP, DEHP, BBP) have become subject to strict regulations because they can act as endocrine disruptors. They can migrate from plastics into the environment, food or cosmetics. For this reason, monitoring their composition and concentration in products is essential.

Various techniques are used to characterize phthalates: IR spectroscopy, useful for identifying functional groups (C=O, C–O, benzene). GC–MS, the standard method for identifying and quantifying individual phthalates in a mixture. HPLC for less volatile compounds. NMR for confirming chemical structure [13, 19].

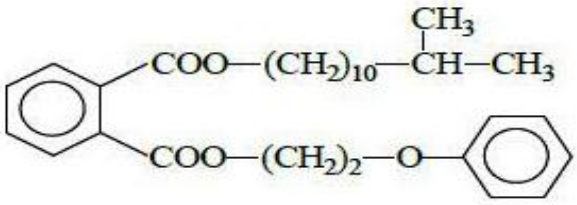
Material and methods

Synthesis of phthalic esters

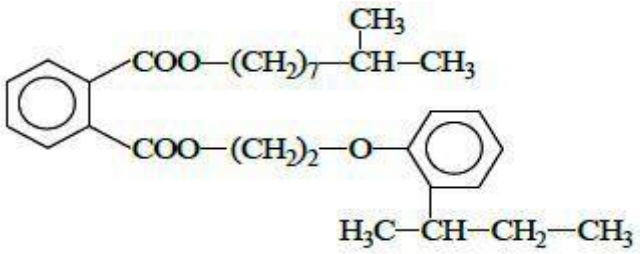
Isodecyl 2-phenoxy ethyl phthalate was obtained by esterification of 1.57 mol of phthalic anhydride with 1.63 mol of isodecanol between 1.63 mol of 2-phenoxy ethanol and 0.037 mol of p-toluene sulfonic acid. The products are obtained according to the procedure in a single step, at a temperature of 100 - 110^{0}C, during 6 - 8 hours, using 170 ml of toluene.



Isotridecyl 2-phenoxy ethyl phthalate was obtained by esterification of 1.25 mol of phthalic anhydride with 1.35 mol of isodecanol between 1.31 mol of 2-phenoxy ethanol and 0.037 mol of p-toluene sulfonic acid. The products are obtained according to the procedure in a single step, at a temperature of 100 - 110^{0}C, during 6 - 8 hours, using 170 ml of toluene.



Isodecyl phthalate and 2-(o-sec-butyl-phenoxy) ethyl were obtained by esterification of 1.250 mol of phthalic anhydride with 1.320 mol of isodecanol between 1.320 mol of 2-(o-sec-butyl-phenoxy) ethanol and 0.037 mol of p-toluene sulfonic acid. The products are obtained according to the procedure in a single step, at a temperature of 100 - 110^{0}C, during 6 - 8 hours, using 170 ml of toluene.



Structure determination

IR spectra were obtained on a Jasco 430 FT-IR spectrophotometer. Samples were prepared in KBr pellets or in film between two KBr panes. FT-IR reactions were monitored in thermostated cuvettes with 0.137 mm thick silicon panes on a Jasco 430 FT-IR spectrophotometer with a resolution of 1 cm^{-1}.

Fig 1: Jasco 430 FT-IR spectrophotometer

Results and discussion

Figure 2 shows the spectrum of isodecyl phthalate and 2-phenoxy ethyl.

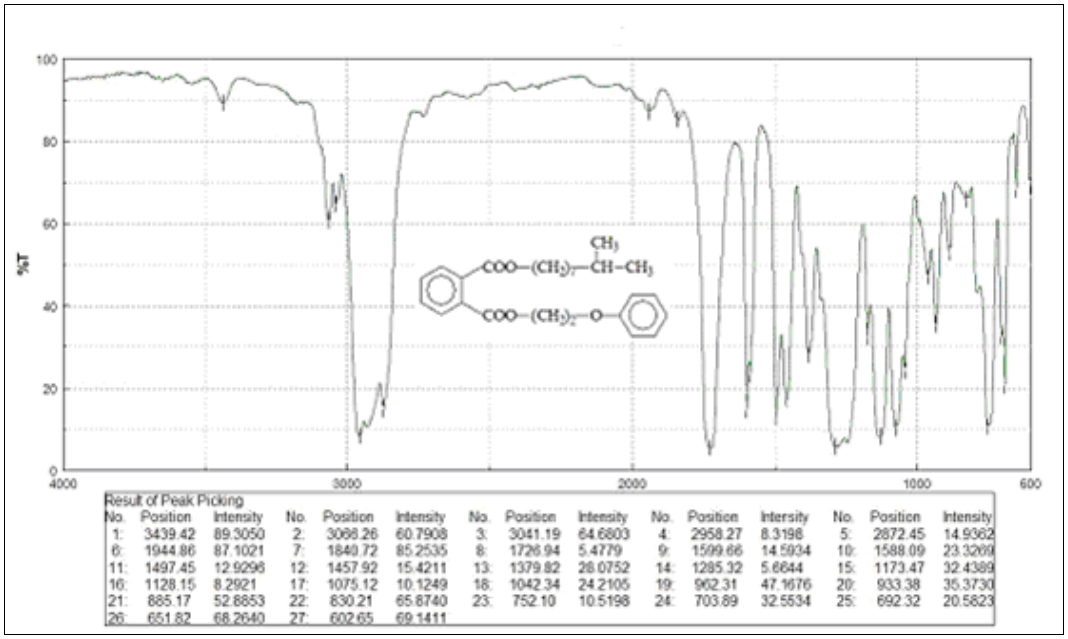


Fig 2: IR spectrum of isodecyl phthalate and 2-phenoxy ethyl

Table 1 shows the assignment of peaks in the FTIR spectrum of isodecyl phthalate and 2-phenoxy ethyl.

Table 1: Assignment of peaks in the FTIR spectrum of isodecyl phthalate and 2-phenoxy ethyl

Wave number, cm^{-1}	Functional grouping	Vibration mode
2958	CH_3 aliphatic	asymmetric
2872	CH_3 flavored	symmetrical intense
1726	C=O, saturated esters	intensity
1599	$\nu_{sch.arom} + \delta_{CH_{intensity}}$	intensity
1497, 1285	$\nu^{s}_{CO(intensity)} + \gamma^{as}_{Ar-C-CH_2(inensity)}$	intensity

Figure 3 shows the spectrum of isotridecyl phthalate and 2-phenoxy ethyl.

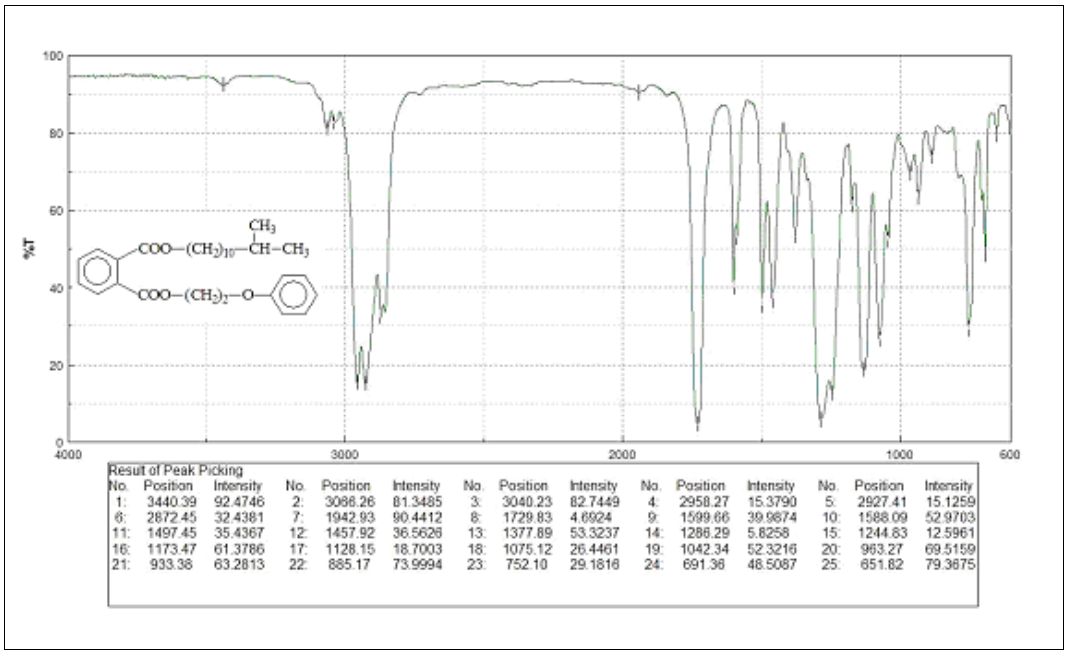


Fig 3: IR spectrum of isotridecyl phthalate and 2-phenoxy ethyl

Table 2 shows the assignment of peaks in the FTIR spectrum of isotridecyl phthalate and 2-phenoxy ethyl.

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Wave number, cm^{-1}	**Functional grouping**	**Vibration mode**
2958	CH_3 aliphatic	asymmetric
2927	CH_3 aliphatic	asymmetric
2872	CH_3 flavored	symmetrical intense
1729	C=O, saturated esters	intensity
1497, 1457, 1286	$\nu^{s}_{CO(intensity)} + \gamma^{as}_{Ar-C-CH_2\,(inensity)}$	intensity

Figure 4 shows the spectrum of isodecyl phthalate and 2-(o-sec-butyl-phenoxy) ethyl..

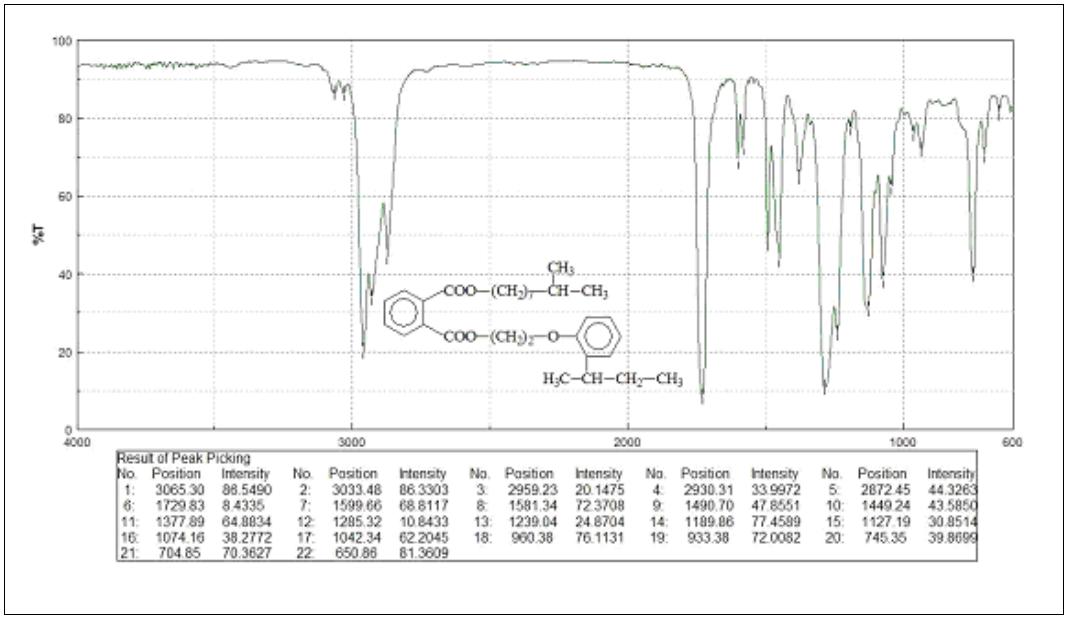

Fig 4: IR spectrum of isodecyl phthalate and 2-(o-sec-butyl-phenoxy) ethyl

Table 3 shows the assignment of peaks in the FTIR spectrum of isodecyl phthalate and 2-(o-sec-butyl-phenoxy) ethyl.

Table 3: Assignment of peaks in the FTIR spectrum of isodecyl phthalate and 2-(o-sec-butyl-phenoxy) ethyl

Wave number, cm^{-1}	Functional grouping	Vibration mode
2959	CH_3 aliphatic	asymmetric
2930	CH_3 flavored	asymmetric
2872	CH_3 flavored	symmetrical intense
1729	C=O, saturated esters	intensity
1285	$\nu^{s}_{CO(intensity)} + \gamma^{as}_{Ar-C-CH_2\,(inensity)}$	intensity

Conclusions

The synthesized phthalic esters are: isodecyl 2-phenoxy ethyl phthalate, isotridecyl 2-phenoxy ethyl phthalate and isodecyl 2-(o-sec-butyl-phenoxy) ethyl phthalate, which have the following functional groups: CH_3, C=O, Ar-C-CH_2 determined with the Jasco 430 spectrometer.

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