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Composition of polyethylene and polypropylene determined by IR spectroscopy

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Abstract
In this article, we determined the composition of polyethylene and polypropylene by FTIR spectroscopy using the IRSpirit-TX FTIR spectrometer. The two polymers have absorption spectra between the wavelengths: 3200 and 720cm^{-1}. The functional groups that enter the composition of the two polymers are: CH, CH_2, CH_3.

Keywords: chemical composition, polyethylene, polypropylene, IR spectroscopy

Introduction

Polyethylene (abbreviated PE) or polymethylene is a white or semi-transparent semi-crystalline thermoplastic polymer, the most widespread plastic material, obtained by the polymerization process, being produced by the petrochemical industry. Annual production in the world is approximately 80 million tons.

Types of polyethylene depending on density, molecular chain construction: PEX or XLPE - cross-linked polyethylene PE-LD - low density polyethylene PE-LLD - low linear density polyethylene (density: 0.915–0.925 g/cm^3). PE-LMD - medium density polyethylene (density: 0.926–0.940 g/cm^3). PE-HD - high density polyethylene 0.97 g/cm^3) PE-HD-HMW - high density polyethylene (high density) with high molecular weight PE-HD-UHMV - high density polyethylene with very high molecular weight, etc [1-5].

Uses: packaging material (plastic bags, membrane, foil, containers, etc.), extruded sheets (which can be milled, thermo-welded, thermoformed), from which composters, doors, industrial screens, self-lubricating gears, shelves, pipes and fittings, foils, bars, sliding elements (in the food industry, gutters, channels). The chemical formula of polyethylene is $(C_2H_4)_n$. From the chemical formula, "n" can take different values, and different plastics are obtained by mixing different types of polyethylene with different "n" values.

The physical properties are: thermoplastic polymer, formed by long hydrocarbon chains. The melting point depends on the type of polyethylene, typical values being in the range of 120 - 130 °C. The melting point for low-density polyethylene for common use is 105 - 115 °C.

The chemical properties are: it has excellent chemical resistance, is resistant to acids, bases, oxides. Polyethylene burns slowly with a blue flame with a yellow tip and gives off a paraffin-like odor. It dissolves in aromatic hydrocarbons such as toluene and xylene or chlorinated solvents.

Polypropylene is a more heat-resistant plastic than polyvinyl chloride (PVC). It is used in the plastics industry, especially in heating systems.

In 2007, the global polypropylene market had a volume of 45.1 million tons, which led to a turnover of 65 billion US dollars (47.4 billion Euros).

Chemical and physical properties are: most commercial polypropylene is isostatic and has an intermediate level of crystallinity between that of low-density polyethylene (LDPE - low-density polyethylene) and that of high-density polyethylene (HDPE - high-density polyethylene). Normal polypropylene is hard and flexible, especially when copolymerized with ethylene. This allows polypropylene to be used as a plastic for automotive production competing with ABS. Polypropylene is inexpensive and can become translucent when uncolored [6-12].

Materials and methods

The instruments used in these measurements were an IRSpirit- TX FTIR spectrophotometer and QATR™-S single-reflection ATR accessory. Fig. 1 show the appearance of the IRSpirit-X series and the measurement conditions, respectively. A diamond prism was used in the QATR-S. A background measurement was carried out with no specimen of any kind on the prism, after which the samples were firmly fixed on the prism and their infrared spectra were acquired.

Fig 1: Appearance of IRSpirit™-X Series

Results and discussions

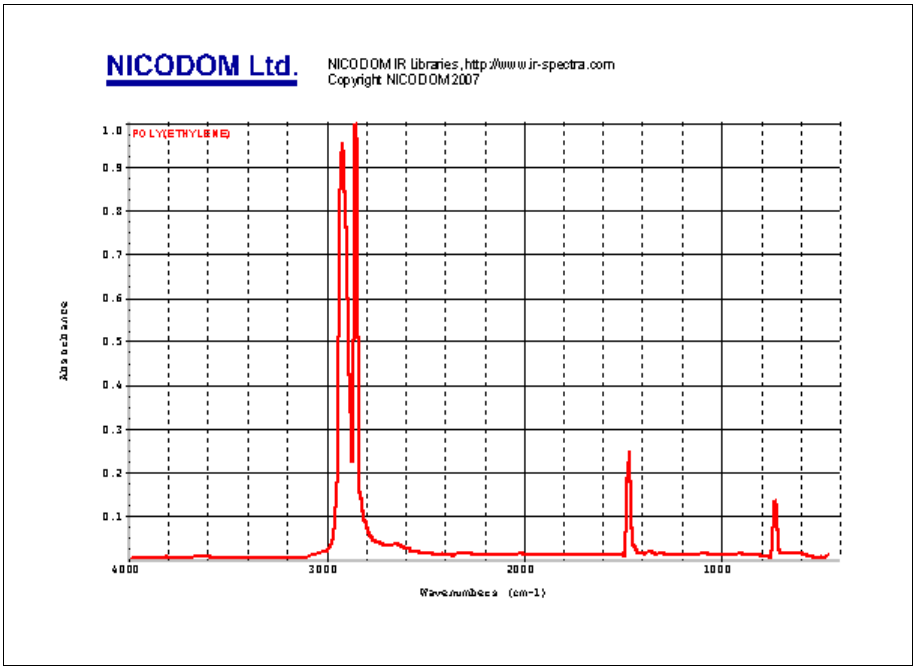

Fig.2: IR spectrum of polyethylene

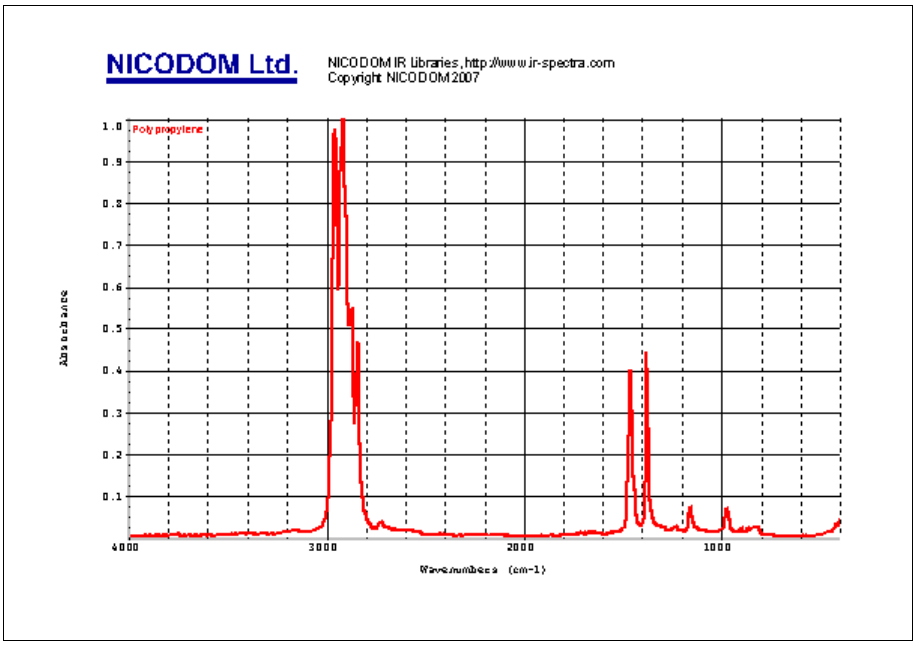

Fig 3: IR spectrum of polypropylene

Infrared spectra of polyethylene and polypropylene were measured using an ATR accessory instrument. Figures 2 and 3 show the measurement results for polyethylene and polypropylene which are indicated by the red line. The absorption related to the C-H stretching vibration can be seen in the vicinity of 3200 to 2600 cm^{-1}, while the absorption related to the C-H bending vibration can be seen in the region in the vicinity of 1600 to 1200 cm-1. The absorption related only to polyethylene can be observed around 720 cm-1.

Absorption originating from the stretching vibration of CH2, a molecule common to polyethylene and polypropylene, can be seen around 2930 cm-1 and around 2850 cm-1. These two peaks show the absorption associated with the asymmetric and symmetric stretching vibration of CH_2, respectively. Although a slight difference in the absorption peak positions of polyethylene and polypropylene can be observed, this is believed to be caused by differences in molecular structure and adjacent CH_2 functional groups.

In addition, from polypropylene, prominent absorption peaks originating from the asymmetric stretching vibration and the symmetric stretching vibration of CH_3 can be recognized around 2960 cm^{-1} and 2870 cm^{-1}, respectively

Although peaks of both polyethylene and polypropylene can be seen around 1460 cm^{-1}, their peak assignments are known to be slightly different. In polyethylene, CH_2 shows a relatively sharp peak originating from the scissor vibration of CH_2. However, in polypropylene, in addition to the scissor vibration of CH_2, a broad peak can be observed due

to the overlap of the absorption peaks of the symmetric CH_3 bending vibration, which is positioned on the side with a somewhat lower wavenumber than the scissor vibration of CH_2. In addition, the prominent peak around 1380 cm^{-1}, which originates from the CH_3 asymmetric bending vibration observed in polypropylene, is also a distinctive feature of polypropylene.

On the other hand, the peak at about 720 cm^{-1} is visible in polyethylene but cannot be observed in polypropylene. This is called the rocking vibration of CH_2. Because the accordion bellows-like stretch can be seen in CH_2-CH_2-CH_2, which is the main chain of polyethylene, it is also called "accordion vibration" as another name.

As demonstrated here, if there are partial differences in the structures of the resins, it is possible to differentiate the type of resin by differences in their infrared spectrum, even in resins consisting only of C and H [13-19].

Conclusions

Polyethylene (abbreviated PE) or polymethylene is a white or semi-transparent semi-crystalline thermoplastic polymer, the most common plastic material, obtained through the polymerization process, being produced by the petrochemical industry.

Polypropylene is a plastic material more resistant to heat than polyvinyl chloride (PVC). It is used in the plastics industry, especially in heating installations. The two polymers have an absorption spectrum between the wavelengths: 3200 and 720cm^{-1} and the functional groups that enter into the composition of the two polymers are: CH, CH_2, CH_3.

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