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# Infrared spectral analysis of waste pet samples

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**ABSTRACT**

There are fifteen waste pet bottles and a commercial grade ABS was collected from local supplier of Chidambaram town. The ABS was used to study the mechanical properties of PET blend composites. This study was performed by FT-IR spectroscopy. From the characteristics infra-red stretching bands the mechanical properties of samples were discussed

**Keywords:**

Pet bottles, ABS, FT-IR Spectra, Blended composites.

## 1. INTRODUCTION

Infrared spectroscopy is a powerful tool technique for studying the qualitative and quantitative analysis [1] of natural and synthetic molecules. IR spectroscopy can provide the information about the nature, concentration and structure of samples at the molecular level [2] in material science. Immense work has been done in the QSAR-LFER and reactivity studies [3] of various organic substrates. Razzak et. al. [4] have studied the end-group determination in poly(ethylene terephthalate) by infrared spectroscopy. In their investigations, the correlations of the hydroxyl and carboxyl units were derived independently for accurate calibration results. The intermediate monomer of PET, bis(hydroxyethyl terephthalate), was used to prepare hydroxyl end-group standards and titration measurements were used to determine the carboxyl content for the carboxyl end-group standards. A double-Gaussian form equation was defined to account for the interference between the hydroxyl and the carboxyl absorbance peaks in the PET IR spectrum. Some deviation was found from the assumption traditionally used for end-group

Determination, stating that carboxyl and hydroxyl are the only end-group units available in PET. The degradation of pet samples by portland cement –based materials was studied by Silva et. al., [5]. During this study the degradation process was monitored by IR spectroscopy and this test was completed after 150 days in alkaline media. An experimental technique and method introduced for measuring carbonation loss in beverage bottles and predicting self-life thereof utilizes infrared absorption spectroscopy [6]. Characterization of crystallinity and degree of crystallinity was studied by Nguyen et.al. through IR spectral analysis [7]. Stretch-blow molding of PET bottles- temperature distribution performance was studied through infrared heating by Bordival et.al. [8]. Kirov and Assender [9] investigates the surface structure of commercial Anisitropic polymer films-PET samples by quantitative

ATR-IR analysis. Mitsuru and Hiroaki [10] introduced the automatic colour identification technique for pet bottles. The concentrations of diethylene glycol (DEG) and iso-phthalate (IPA) units present in two commercial polyesters were measured using Fourier transform infrared (FTIR) spectroscopy and by a lowering of the melting point as measured by differential scanning calorimetric (DSC) method [11]. The properties of metal blended terephthalates were studied through differential thermal analysis and IR spectroscopy [12].

In order to recyclization of polymeric materials, the polymer identification techniques and analysis of additives are required. Economic aspects demand fast response times, easy handling and integration in automated or at least semi-automated systems. As macroscopic physical methods, e.g. those based on density measurements, are not sufficient to separate polymers, identification has to use methods monitoring structural or molecular properties of the polymer under investigation [13]. A number of techniques have been developed to assist in identification of polymers. They are: Near Infrared Spectroscopy [14, 15, 16] Direct Pyrolysis Mass spectrometry [17], Electrostatic method: Triboelectric [18], X-ray Spectroscopy [19] and Chemical Recycling [20]. However, none of these methods has proved to be either completely satisfactory or acceptable in dealing with a wide proportion of the polymer waste. The most recent developed technique, Broadband Ultrasound Attenuation analysis, is a versatile technique that can be applied to a wide variety of material analysis applications. In this article the authors have to take effort for collection of some waste pet bottle and ABS recorded their FT-IR spectra and studied the characterization.

## 2. EXPERIMENTAL DETAILS

### 2.1. Collection of materials

Waste PET bottles from a local supplier of Chidambaram town were used in the present work. A commercial grade of ABS was used to study the mechanical properties for ABS/waste PET blend compositions.

### 2.2. Blending

The required quantities of ABS and waste PET were dried at 100-120 ºC for 6 hours in an air circulating oven before dry blending. The blend was prepared via melt compounding method using twin-screw extruder (Bersforft, FRG Germany) at temperature range of 200 ºC to 220 ºC with screw speed of 150 rpm. After extrusion, the extrudate was cooled in a water bath and palletized. The basis of formulation was based on the percentage weight ratio between ABS and waste PET. The outline of different weight ratios of blends are shows in Table 1.

**Table 1:** The weight percentage ratios of ABS and waste Pets

| Blend | Weight percentage of ABS | Weight percentage of waste PET |
|---|---|---|
| I | 100 | 0 |
| II | 97 | 3 |
| III | 94 | 6 |
| IV | 90 | 10 |

## 2.3. FT-IR spectra

Infrared spectra of various waste PET bottle samples was carried out using Thermo Electron Corporation, USA, spectrometer, NICOLET 6700 at a resolution of 4 $cm^{-1}$ at room temperature. For recording IR Spectra, the PET samples were cut into small pieces.

Direct IR spectra recorded on the solid samples. The assigned infrared stretches are tabulated in Table 2.

**Table 2:** Infrared spectroscopic ν ($cm^{-1}$) data of waste pet bottles

| **Band name of PET bottle** | **Ar C-H Wagg.** | **Ar C-H *out of plane*** | **C-H Bend. *in-plane*** | **O-C-C Asymm.** | **C-C-O Asymm.** | **C-H def. in alkane** | **C-H def. in alkane** | **C-H bending** | **Ar C-C bond** | **C=O Ester** | **C-H Asymm.** | **O-H band** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Diet aqua** | 722.5 | 871.9 | 1016.6 | 1093.8 | 1243.0 | 1339.7 | 1408.0 | 1455.4 | 1505.3 | 1713.8 | 2922.6, 2960 | 3,300.0 |
| **Bisvind** | 722.1 | 871.6 | 1014.4 | 1094.4 | 1234.1 | 1339.5 | 1407.9 | 1455.7 | 1505.4 | 1713.8 | 2958.5, 2923 | 2,958.5 |
| **Aquafina** | 722.1 | 871.8 | 1016.4 | 1092.9 | 1241.3 | 1338.9 | 1407.9 | 1455.5 | 1505.0 | 1713.7 | 2923.7, 2960 | 3,380.3 |
| **Kinley water** | 722.1 | 871.6 | 1016.7 | 1093.9 | 1242.0 | 1339.1 | 1408.1 | 1455.8 | 1505.5 | 1713.1 | 2925.6, 2960 | 3,430.6 |
| **Bisleri** | 722.1 | 871.6 | 1016.1 | 1092.7 | 1239.7 | 1338.4 | 1407.9 | 1455.7 | 1505.6 | 1712.9 | 2921.7, 2960 | 3,375.8 |

| **Band name of PET bottle** | **Ar C-H Wagg.** | **Ar C-H *out of plane*** | **C-H Bend. *in-plane*** | **O-C-C Asymm.** | **C-C-O Asymm.** | **C-H def. in alkane** | **C-H def. in alkane** | **C-H bending** | **Ar C-C bond** | **C=O Ester** | **C-H Asymm.** | **O-H band** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Sprite** | 722.5 | 872.0 | 1015.4 | 1091.8 | 1239.0 | 1338.1 | 1407.7 | 1456.0 | 1505.6 | 1713.8 | 2921.5, 2960 | 3,317.6 |
| **Maaza mango** | 722.3 | 871.5 | 1016.6 | 1093.8 | 1241.3 | 1339.0 | 1408.4 | 1455.2 | 1505.2 | 1714.0 | 2963.6, 2923 | 3,400.0 |
| **Fanta** | 722.1 | 871.5 | 1016.2 | 1092.6 | 1239.8 | 1339.2 | 1408.0 | 1455.6 | 1505.4 | 1712.8 | 2922.0, 2960 | 3,400.0 |
| **7-up** | 721.6 | 871.8 | 1015.9 | 1092.1 | 1239.3 | 1338.6 | 1407.8 | 1455.6 | 1505.0 | 1713.0 | 2923.0, 2960 | 3,300.0 |
| **Coco cola** | 722.1 | 871.5 | 1016.3 | 1093.0 | 1239.5 | 1338.9 | 1408.2 | 1455.3 | 1505.0 | 1714.2 | 2920.6, 2960 | 3,400.0 |
| **Pepsi** | 722.5 | 871.8 | 1016.5 | 1093.3 | 1240.1 | 1338.6 | 1408.0 | 1455.6 | 1505.5 | 1713.2 | 2961.5, 2923 | 3,400.0 |
| **Miranda** | 721.3 | 871.3 | 1014.3 | 1087.3 | 1234.1 | 1338.4 | 1407.6 | 1456.1 | 1505.8 | 1712.3 | 2918.4, 2960 | --- |

| Band name of PET bottle | Ar C-H Wagg. | Ar C-H *out of plane* | C-H Bend. *in-plane* | O-C-C Asymm. | C-C-O Asymm. | C-H def. in alkane | C-H def. in alkane | C-H bending | Ar C-C bond | C=O Ester | C-H Asymm. | O-H band |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Slice** | 722.3 | 871.8 | 1015.9 | 1087.2 | 1238.2 | 1338.3 | 1407.9 | 1455.8 | 1504.6 | 1713.4 | 2960.7, 2925 | 3,297.3 |
| **Frooti** | 722.4 | 871.7 | 1016.4 | 1093.8 | 1240.5 | 1338.9 | 1408.2 | 1455.6 | 1505.3 | 1713.5 | 2961.9, 2923 | 3,400.0 |
| **Jaldehara** | 722.5 | 872.3 | 1015.0 | 1090.0 | 1238.7 | 1337.5 | 1407.6 | 1455.9 | 1504.9 | 1713.3 | 2959.1, --- | --- |

## 3. RESULTS AND DISCUSSION

### 3.1. IR spectral study

Infrared spectrum is known to contain information at the molecular level of the material i.e. microstructure. The microstructure is a representation of the characteristics of the material, whether it is chemical (or) physico – mechanical. It may be noted that breadth and shape of the infrared bands are representation of the manner in which molecules relax from the vibrationally excited state reach upon the absorption of an (infrared) photon. The relaxation is known to be achieved through intramolecular and inter molecular non – radiative path ways. These in turn could be considered as an indirect representation of the mechanical properties of the material. The FT-IR Spectra of PET confirms the presence of a carbonyl group in conjugation with aromatic ring appear at 1713 $cm^{-1}$. The second strongest peak at 1234 $cm^{-1}$ is due to the asymmetric c-c-o stretching involving the carbon in aromatic ring. The aromatic C-H wagging appears at 721.8 $cm^{-1}$. The peak at 871.5$cm^{-1}$ corresponds to aromatic C-H out of plane bending. The O-C-C asymmetric stretching is split at 1128 and 1091 $cm^{-1}$. There are also peak at 2960 $cm^{-1}$ (C-H asymmetric stretching) 1505 $cm^{-1}$ (aromatic C-C stretching), 1453 $cm^{-1}$ (C-H bending). Peak at 1408$cm^{-1}$ and 1339$cm^{-1}$ is due to deformation C-H alkane. For the present study following waste PET bottle samples containing respective mineral water or soft drink as given in Table 2. From the table the vibrational frequencies of assigned groups are vary from 0.5- 1.5 $cm^{-1}$ averagely.

### 3.2. Migration test

This is the method of analysis for determination of overall migration of constituents of plastic materials intended to come in contact with food stuffs. The determination of migration in stimulants was carried out using the following stimulants.

- Stimulant A – distilled water.

- Stimulant B – 3% acetic acid w/v in aqueous solution using stimulant A.
- Stimulant C – 10% ethanol (v/v) in aqueous solution using stimulant A.
- Stimulants A was used for aqueous, non-acidic food ($p^H$>5) without fat, like honey, mineral water, sugar syrup molasses, skimmed milk etc.,
- Stimulant B was used for aqueous acidic foods ($p^H \leq 5$) without fat like fruit juices, jams, vinegar, carbonated beverages, lemonade, soups, sauces etc.,

Stimulants C were used for alcoholic beverages like beer and some pharmaceutical syrups. Stimulants equal to normal filling capacity considered. The test was conducted as follows. The Container was filled to capacity with the stimulants and closed and maintained in water bath for the specified duration of time. After exposure for the specified duration, container was removed and contents transferred to a clean beaker along with washings of the specimen with small quantity of the fresh stimulant. Contents of the beaker is evaporated to about 50 – 60 ml and transferred to a cleaned stainless steel dish and further evaporated to dryness in an oven at 100±5 ºC. Dish was cooled and weighed. Extractive was measured in mg/l of the food stuff with respect to the capacity of the container used and it is calculated as follows. *Amount of Extractive = M/V 1000 mg*

Where M = mass of residue in mg subtracted by blank value, V = total volume in ml of stimulant used. The results of migration tests of waste pets are summarized in Table 3. The material were regarded as conforming to the specifications of the migration test for each stimulant used if the value does not exceed the value of overall migration limit specified in the relevant standards.

**Table 3**: Migration test values of waste PET bottles samples.

| S. No | Brand name used on the waste PET bottle | Migration test values in mg/lit for stimulant "A" water | Migration test values in mg/lit for stimulant "B" 3% acetic acid | Migration test values in mg/lit for stimulant "C" 10% alcohol |
|---|---|---|---|---|
| 1 | Diet aqua | 11 | 14 | 12 |
| 2 | Bisvind | 18 | 22 | 17 |
| 3 | Aquafina | 15 | 18 | 14 |
| 4 | Kinley water | 13 | 14 | 13 |
| 5 | Bisleri | 20 | 16 | 18 |
| 6 | Sprite | 18 | 17 | 15 |
| 7 | Maaza mango | 17 | 18 | 22 |
| 8 | Fanta | 21 | 19 | 24 |
| 9 | 7-up | 19 | 18 | 22 |
| 10 | Coco cola | 17 | 20 | 18 |
| 11 | Pepsi | 24 | 22 | 20 |
| 12 | Miranda | 20 | 19 | 16 |
| 13 | Slice | 19 | 21 | 24 |
| 14 | Frooti | 18 | 20 | 25 |
| 15 | Jaldehara | 22 | 11 | 14 |

## 4. CONCLUSION

Exactly fifteen waste pet bottles and a commercial grade ABS were collected from local supplier of Chidambaram town. The ABS was used to study the mechanical properties of PET blend composites. This study was performed by FT-IR spectroscopy. From the spectral analysis all pet bottles gave the characteristic peaks with the variation range 0.5 to 1.5 $cm^{-1}$. From the characteristics infra-red stretching bands the mechanical properties of samples studied with three solvent such as water, acetic acid and alcohol.

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