



## **CASE STUDY**

### **FTIR for Identification of Contamination**

#### **PROBLEM**

The objective of this study is to highlight the ability of FTIR to detect inconsistencies, including percent level contamination or degradation in a material.

#### **ANALYTICAL STRATEGY**

FTIR is sensitive to any component at a concentration of roughly 5% or greater, thus the technique is generally applied for identification of the polymer type but not the additives package or other minor sample components.

#### **CONCLUSIONS**

By analyzing a known polyolefin standard as a comparison, it is identified that contamination is present in the sample.

PYMS is a more powerful technique for identifying unknowns within a particular polymer family or identifying any low-concentration additives or impurities. FTIR is a great method for quick identification of the functional groups present in an unknown sample, but PYMS analysis can provide a much greater level of information and should be the method of choice when this type of information is preferred.

Read the following report to see the full analysis.



# Final Report

Jordi Labs LLC  
Case Study  
FTIR for Identification of Contamination

Date: xx/xx/xx

Released by:  
Dr. Mark Jordi  
President  
Jordi Labs LLC

Report Number: Jxxxx

Company Name Confidential





Date

Client Name

Company Name

Address

Dear Valued Client,

Please find enclosed the test results for your samples described as:

1. Lot# 20110613-CTIW
2. Polyethylene Reference

The following test was performed:

1. Fourier Transform Infrared Spectroscopy (FTIR)

## Objective

The objective of this work was to confirm that the chemistry of your sample is consistent with Polyethylene by Fourier Transform Infrared Analysis.

## Summary of Results

The sample showed a spectrum which was most consistent with a Polyethylene blend. Spectrums of Polyethylene contain four strong bands located at 2916, 2848, 1472 and 716  $\text{cm}^{-1}$ . The Lot# 20110613-CTIW sample contains these four bands and additional bands which can be seen in **Table 1**. The additional peaks are known to be characteristic of Polypropylene. A peak at 1718  $\text{cm}^{-1}$  is consistent with oxidation which may be occurring during processing.

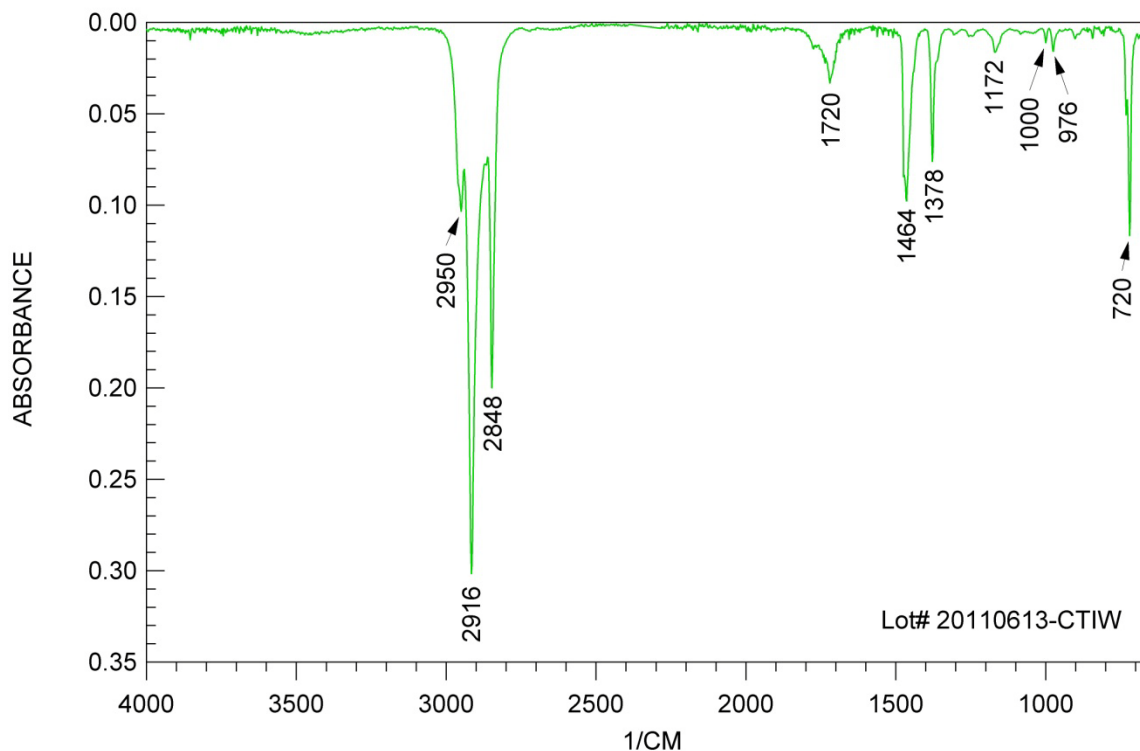
## Individual Test Results

A summary of the individual test results is provided below. All accompanying data, including spectra, has been included in the data section of this report.

### FTIR

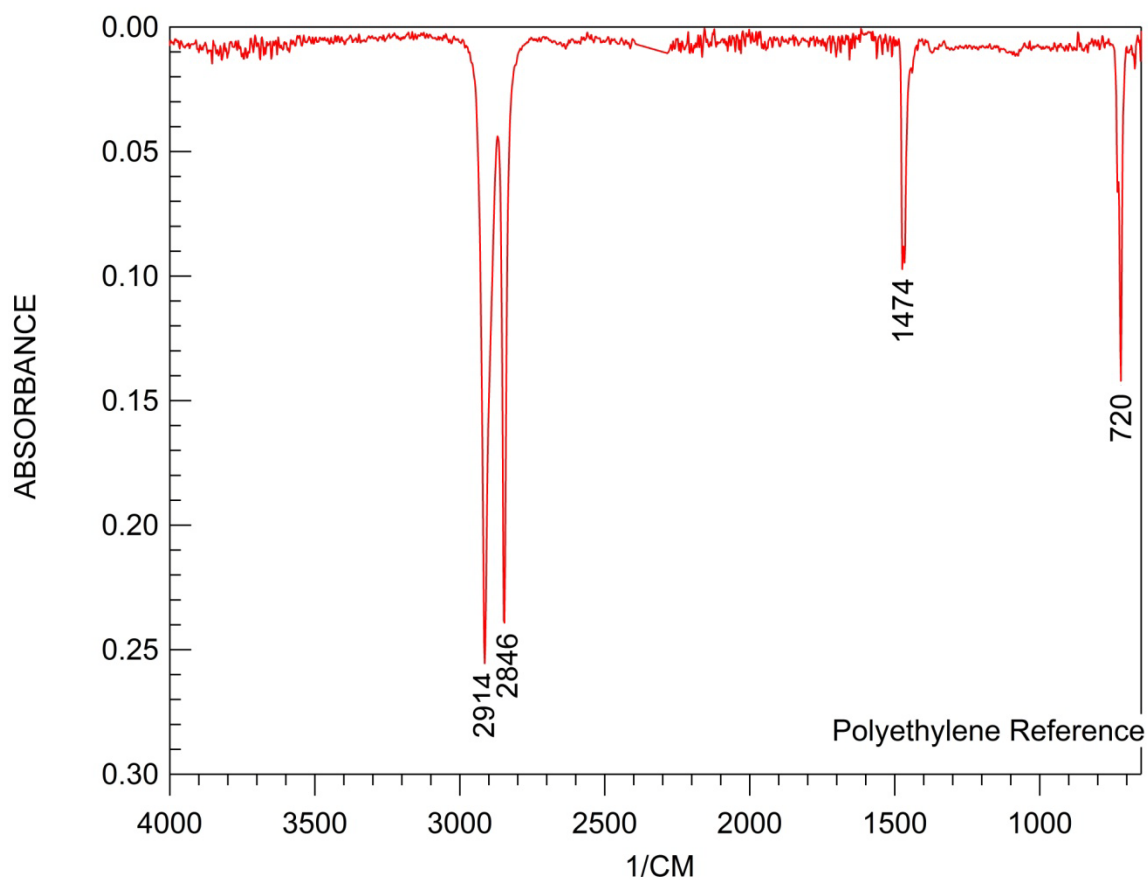
The sample spectrum was compared to our library database of ~20,000 entries and found to be most consistent with Polyethylene, however additional peaks are observed. The additional peaks are consistent with Polypropylene. **Table 1** shows the spectrum peaks and their most probable identifications.

The FTIR spectrum for Lot# 20110613-CTIW is shown in **Figure 1**. Reference spectra for Polyethylene and Polypropylene standards are shown in **Figures 2 and 3** for comparison. **Figure 4** is an overlay of all three spectra.



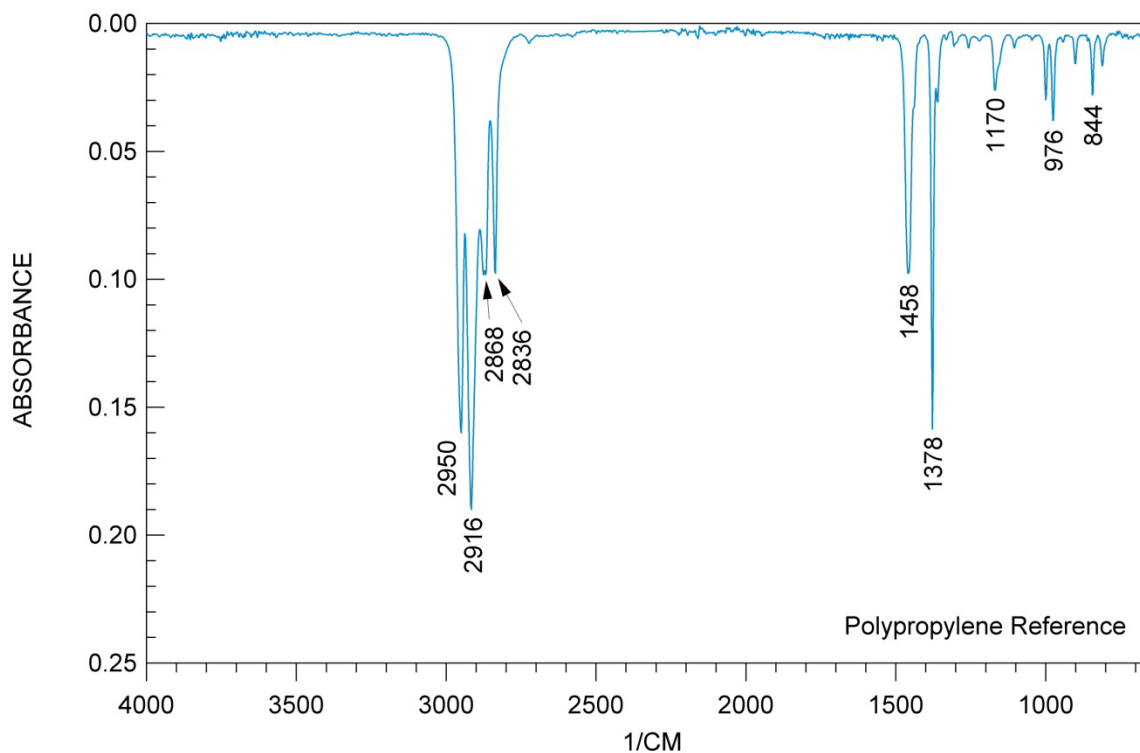
**Figure 1.** FT-IR Spectrum for Lot# 20110613-CTIW

<b>Table 1.</b> <b><i>FTIR Peaks and Identifications for Lot# 20110613-CTIW</i></b>	
<b>IR Frequency (cm<sup>-1</sup>)</b>	<b>Functional Group</b>
2950	CH Stretch (PP)
2916, 2848	CH Stretch (PE)
1720 (weak)	C=O Stretch (Possible Oxidation)
1464	CH <sub>2</sub> Deformation/CH <sub>2</sub> Bend (PP and PE)
1378	Symmetric CH <sub>3</sub> Deformation (PP)
1172, 1000, 976	Isotactic Polypropylene Bands (PP)
720	CH <sub>2</sub> Rock (PE)



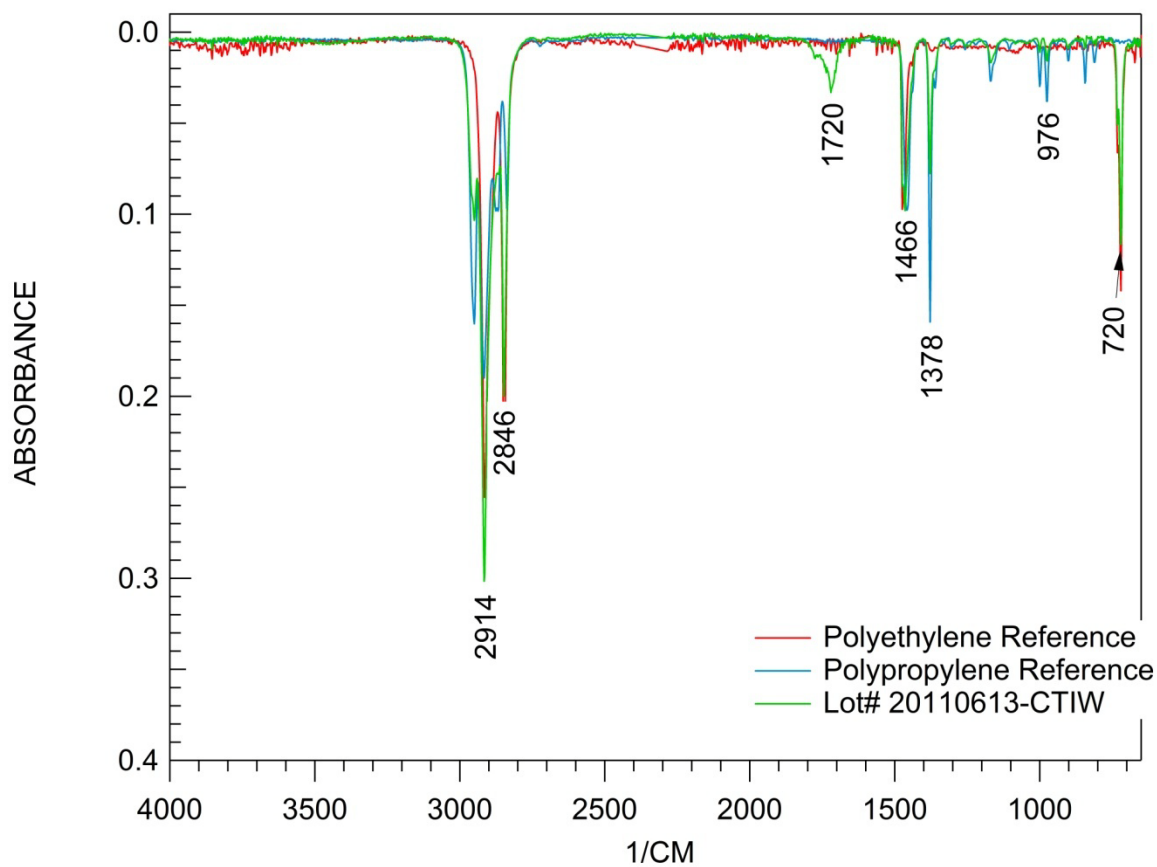
**Figure 2.** FT-IR Spectrum of Polyethylene Reference.

Table 2. <i>FTIR Peaks and Identifications for Polyethylene Reference</i>	
IR Frequency (cm <sup>-1</sup> )	Functional Group
2914, 2846	CH <sub>2</sub> stretch
1474	CH <sub>2</sub> bend
720	CH <sub>2</sub> rock

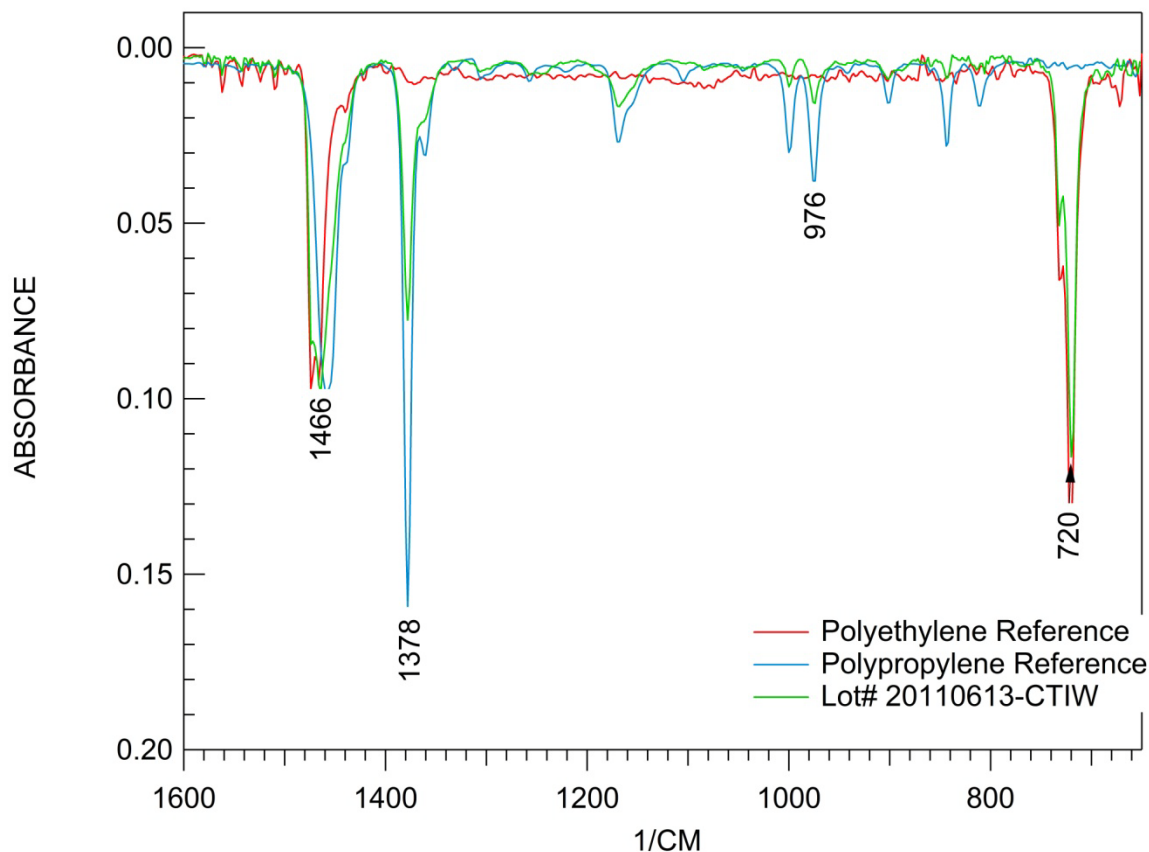


**Figure 3.** FT-IR Spectrum of Polypropylene Reference

Table 3. <i>FTIR Peaks and Identifications for Polypropylene Reference</i>	
IR Frequency (cm <sup>-1</sup> )	Functional Group
2950, 2918, 2836	CH Stretch
1456	CH <sub>2</sub> Deformation
1376	Symmetric CH <sub>3</sub> Deformation
1166	Isotactic Polypropylene Band
998	Isotactic Polypropylene Band
974	Isotactic Polypropylene Band
842	Isotactic Polypropylene Band



**Figure 4.** FT-IR Spectrum Overlay of Lot# 20110613-CTIW, Polyethylene and Polypropylene



**Figure 5.** Zoom of FT-IR Spectrum Overlay of Lot# 20110613-CTIW, Polyethylene and Polypropylene

## Analysis Conditions

### FTIR

A portion was removed from your sample using a clean razor and tweezers and was tested as-is on a Perkin-Elmer PC-16 FT-IR spectrometer fitted with a DuraScope diamond ATR system (an integrated video imaging accessory). The DuraScope is designed for the analysis of all sample types. The spectrum generated by the sample was compared to ~ 20000 entries in our library and the best match determined based upon absorbencies and peak intensities.

### Closing Comments

Deformation of an unknown material is intended to provide a best estimate of the chemical nature of the sample. All chemical structures are supported by the evidence presented but are subject to revision upon receipt of additional evidence. Additional factors such as material processing conditions may also affect final material properties.



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Jordi Labs specializes in polymer testing and has 30 years experience doing complete polymer reformulations. We are one of the few labs in the country specialized in this type of testing. We will work closely with you to help explain your test results and solve your problem. We appreciate your business and are looking forward to speaking with you concerning these results.

Sincerely,

*Laurie Scharp*

Laurie Scharp  
Chemist  
Jordi Labs LLC

*Mark Jordi*

Mark Jordi, Ph. D.  
President  
Jordi Labs LLC

# FTIR Data

