Rapid Screening of Virgin and Recycled Polymer Resins Using FTIR and Raman Libraries of Pre-computed Mixture Spectra

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Overview

Purpose: Screening plastics with ATR/FTIR and Raman libraries designed for plastic analysis.

Methods: ATR/FTIR and Raman

Results: Effective multicomponent plastic identification

Introduction

The FDM ATR Plastics Kit and the FDM Raman Plastics Kit are spectral libraries designed to rapidly screen plastics. ATR/FTIR and Raman spectra of neat polymer resins, inorganic fillers, plasticizers, and polymer additives were selected and digitally combined to render mixture spectra. Using either library avoids (a) the time and expense of planning, preparing and running multicomponent standards and (b) time consuming and computationally intensive multi-component searches. The application of the libraries described here shows rapid and effective screening of real-world plastic materials. No quantitative calibration was required. The percentages are estimates of relative con-centration. The results can guide further analysis. The ATR/FTIR and Raman results are independent of each other.

Experimental

All FTIR spectra were run using a PIKE GladiATR with a monolithic diamond ATR crystal and a Bruker Equinox FTIR, with N_2 purge, over the range of 4000 to 400 cm^{-1}. No baseline correction was performed. Optical resolution was 2 cm^{-1}.

All Raman spectra were run on a Thermo DXR SmartRaman™ with a 300 mW, 780 nm laser. White light correction and autoexposure were used to produce spectra of optimal quality. The spectral range was 3200 to 200 cm^{-1}. Baseline correction was performed manually. Optical resolution was nominally 4.3 cm^{-1} at 1000 cm^{-1}.

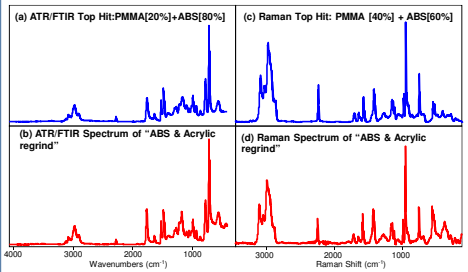
Analysis

The searching operations described were simple. No spectral ranges were specified meaning the full range of the sample spectra were searched against the library. The search algorithms were either correlation coefficient or first derivative correlation coefficient.

DISCUSSION: Binary Mixture

A sample labelled “ABS and Acrylic regrind” was obtained. The ATR/FTIR and Raman spectra were searched. Figure 1 shows the identification and estimated relative concentrations of ABS and PMMA. Note the Raman results do not cluster as well as the ATR/FTIR results . This is likely due to the fact that FTIR absorbance is more linear with concentration than the Raman effect. ATR/FTIR sampling and data processing are less subjective than with Raman. Nevertheless, both top hits offer visually compelling suggestions as to the mixture components.

FIGURE 1: ABS and Acrylic regrind. (a) and (c) (blue) are library spectra. (b) and (d) (red) are sample spectra.

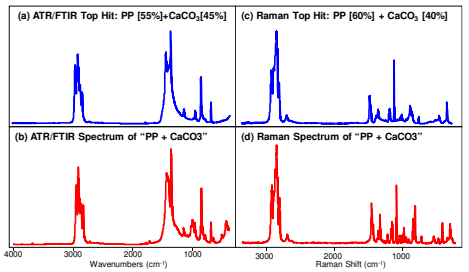


ATR/FTIR		Raman	
Score	Name	Score	Name
0.9683	PMMA [20%] + ABS [80%]	0.9423	PMMA [40%] + ABS [60%]
0.9678	PMMA [25%] + ABS [75%]	0.9416	PMMA [35%] + ABS [65%]
0.9652	PMMA [15%] + ABS [85%]	0.9390	PMMA [45%] + ABS [55%]
0.9626	PMMA [30%] + ABS [70%]	0.9385	PMMA [40%] + SAN [60%]
0.9529	PMMA [25%] + SAN [75%]	0.9367	PMMA [30%] + ABS [70%]
0.9518	PMMA [5%] + ABS [95%]	0.9360	PMMA [45%] + SAN [55%]
0.9516	PMMA [20%] + SAN [80%]	0.9360	PMMA [35%] + SAN [65%]

DISCUSSION: Polymer with Filler

A sample labeled “Polypropylene + Calcium Carbonate” was obtained. The ATR/FTIR and Raman spectra were searched. Figure 2 shows the identification and estimated relative concentrations of PP and $CaCO_3$. Again the results differ but both are clearly useful for screening. Note the small unmatched peaks in the fingerprint regions of both sample spectra (red). This shows libraries of mixture spectra can be useful when minor components are present. In the ATR/FTIR spectrum, an analyst might perform further searching on just the peaks around 1000 cm^{-1} since they can be confident it is neither PP or $CaCO_3$.

FIGURE 2. Polypropylene and $CaCO_3$. (a) and (c) (blue) are library spectra. (b) and (d) (red) are sample spectra.

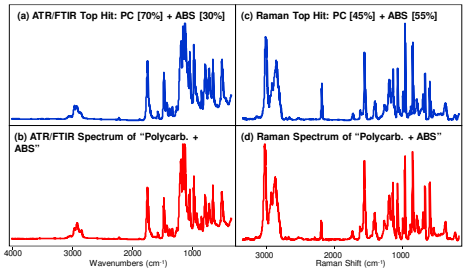


ATR/FTIR		Raman	
Score	Name	Score	Name
0.9602	PP [55%] + $CaCO_3$ [45%]	0.9689	PP [60%] + $CaCO_3$ [40%]
0.9584	PP [50%] + $CaCO_3$ [50%]	0.9686	PP [65%] + $CaCO_3$ [35%]
0.9555	PP [60%] + $CaCO_3$ [40%]	0.9674	PP [70%] + $CaCO_3$ [30%]
0.9504	PP [45%] + $CaCO_3$ [55%]	0.9674	PP [55%] + $CaCO_3$ [45%]
0.9440	PP [65%] + $CaCO_3$ [35%]	0.9655	PP [75%] + $CaCO_3$ [25%]
0.9371	PP [40%] + $CaCO_3$ [60%]	0.9635	PP [50%] + $CaCO_3$ [50%]
0.9262	PP [70%] + $CaCO_3$ [30%]	0.9632	PP [80%] + $CaCO_3$ [20%]

DISCUSSION: Pellet Blend with Colorant

A sample of brown plastic pellets labelled as a blend of Polycarbonate (PC) and Acrylonitrile Butadiene Styrene (ABS) was obtained. The spectra where searched. Figure 3 shows the identification and estimated relative concentrations of PC and ABS. Again we see good results even when other minor components, in this case an unknown brown pigment, are present .

FIGURE 3. Polycarbonate and ABS. (a) and (c) (blue) are library spectra. (b) and (d) (red) are sample spectra.



ATR/FTIR		Raman	
Score	Name	Score	Name
0.9398	PC [70%] + ABS [30%]	0.9080	PC [45%] + ABS [55%]
0.9377	PC [75%] + ABS [25%]	0.9076	PC [50%] + ABS [50%]
0.9368	PC [65%] + ABS [35%]	0.9042	PC [40%] + ABS [60%]
0.9354	PC [75%] + SB [25%]	0.9038	PC [55%] + ABS [45%]
0.9327	PC [70%] + SB [30%]	0.8971	PC [60%] + ABS [40%]
0.9327	PC [70%] + SAN[30%]	0.8958	PC [35%] + ABS [65%]
0.9326	PC [75%] + SAN [25%]	0.8953	PC [45%] + SAN [55%]

Conclusion

Rapid and effective screening of plastic samples was accomplished with little effort using both the **FDM ATR Plastics Kit** and the **FDM Raman Plastics Kit** spectral libraries.