Application Note

Materials

Accurate Identification of Binder Raw Materials for Li-Ion Battery Electrodes by FTIR

Rapid quality control of incoming materials using the Agilent Cary 630 FTIR

Authors

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Abstract

With the rapid growth of lithium-ion battery manufacturing driven by the global push towards cleaner energy technologies, maintaining strict quality control of raw materials is more critical than ever. Even materials that are used in small quantities, such as binders, are important since they ensure mechanical integrity, electrochemical performance, and long-term reliability of battery electrodes. Variations in binder composition or quality can significantly impact manufacturing yield and battery performance. This application note demonstrates how the Agilent Cary 630 FTIR spectrometer, combined with Agilent MicroLab software, provides a fast, reliable, and easy-to-use method for identifying and verifying binder materials in incoming raw material streams.

Introduction

Lithium-ion battery (LIB) production relies on a wide variety of specialized materials sourced from numerous suppliers. In high-throughput LIB manufacturing facilities, even minor inconsistencies in raw materials can lead to significant downstream effects on cell performance. Binders are a good example: although used in small quantities to adhere active materials to metal current collectors, they are critical to electrode functionality. Binders directly influence electrode mechanical strength, uniformity, and long-term cell performance. As a result, production engineers and quality control (QC) managers consider binder verification as a key part of quality assurance (QA) workflows.

Traditional binders such as polyvinylidene fluoride (PVDF) are effective but introduce environmental and solvent-handling concerns. Alternatives such as polytetrafluoroethylene (PTFE), styrene-butadiene rubber (SBR), and carboxymethyl cellulose (CMC) are increasingly being adopted within the industry to align with evolving sustainability standards. However, these changes also introduce new risks for LIB manufacturers — particularly when material specifications vary or supply sources change. To maintain production consistency and reduce the risk of batch failure or rework, fast and accurate material identification and verification tools are needed. FTIR spectroscopy offers a simple yet powerful solution for the QA/QC of various LIB raw materials. Given the organic and polymeric nature of binders, FTIR spectroscopy offers a rapid and reliable means of identifying them, as discussed in the "Characterization of PVDF polymorphic phases" section of this application note.

This study outlines how the Agilent Cary 630 FTIR spectrometer (Figure 1) with its compact footprint can be used at the point of material receipt to verify binder identity. User-friendly Agilent MicroLab software ensures successful operation following minimal operator training. Analyses carried out using the Cary 630 FTIR support fast decision-making, help avoid production disruptions, and improve end-product reliability.

Figure 1. The Agilent Cary 630 FTIR spectrometer. With its ultra-compact design (footprint of 20 × 20 cm and weighing only 3.6 kg), the Cary 630 FTIR can easily be used where needed to produce high-quality results for incoming LIB raw materials.

Experimental

Workflow

The development and testing of a routine LIB-binder-material identification method is shown in Figure 2.

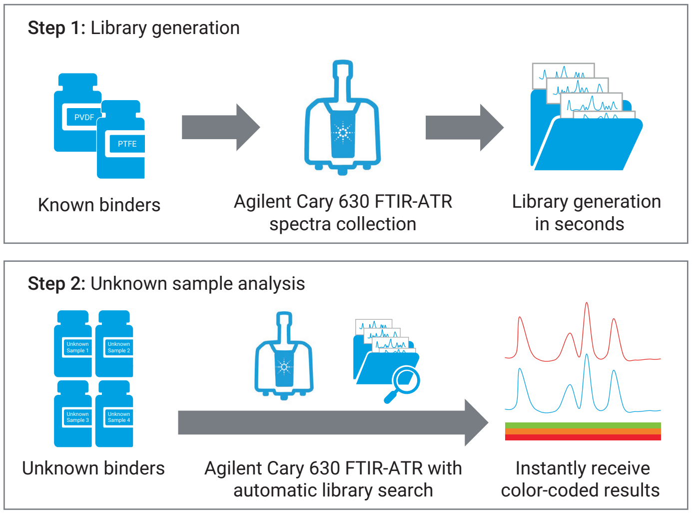

Figure 2. Workflow for identification of LIB binders using an Agilent Cary 630 FTIR and Agilent MicroLab software.

Instrumentation and library-creation

As shown in Step 1 of the workflow, a Cary 630 FTIR spectrometer equipped with an Agilent diamond ATR module was used in this study. The instrument was used to create a "user-generated LIB binders" spectral reference library for two binder materials, PVDF and PTFE. Both "reference" materials were from SP2 Scientific Polymer Products Inc (New York, USA). The spectral acquisition parameters are detailed in Table 1.

Table 1. Agilent Cary 630 FTIR-ATR operating parameters.

Parameter	Setting
Method	Library search
Library Used	User-generated LIB binders library
Search Algorithm	Similarity
Spectral Range	4,000 to 650 cm^{-1}
Background Scans	32
Sample Scans	32
Spectral Resolution	4 cm^{-1}
Background Collection	Air
Zero Fill Factor	None
Apodization	HappGenzel
Phase Correct	Mertz
Color-Coded Confidence Level Thresholds	Green (high confidence): > 0.95 Yellow (medium confidence): 0.91 to 0.95 Red (low confidence): < 0.91

Samples

As shown in Step 2 of the workflow, four binders were analyzed as "unknowns" using the parameters listed in Table 1. The samples included three PVDF binders and one PTFE binder, all bought from TOB Company (Tong'an District, Xiamen City, Fujian Province, China).

Software

The Cary 630 FTIR spectrometer was operated using Agilent MicroLab software. The software features an intuitive, pictorial interface that guides users through the analysis process—from sample introduction to data acquisition and final reporting (Figure 3).

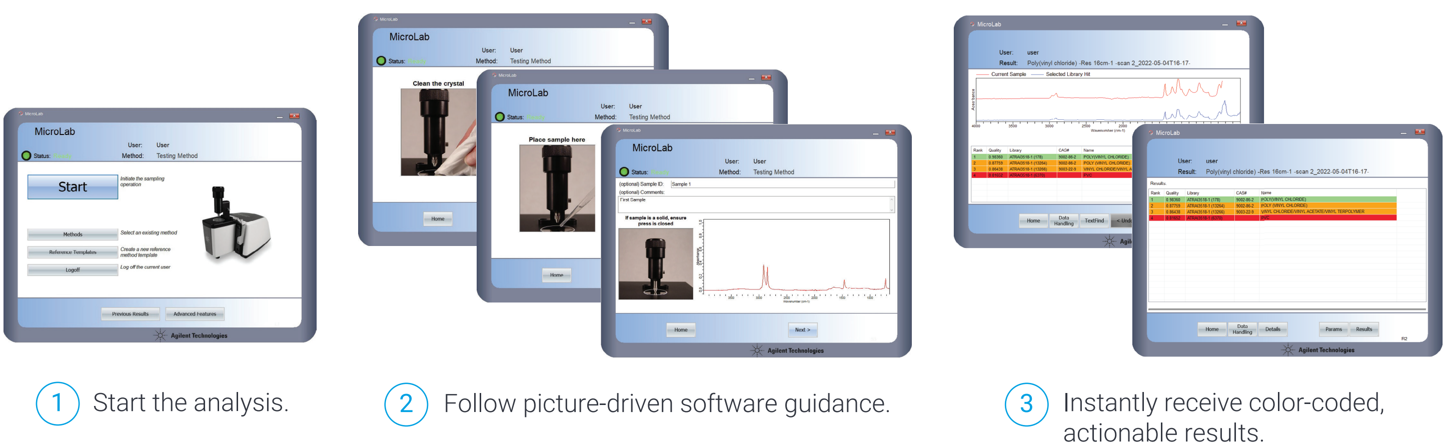

Figure 3. Agilent MicroLab software simplifies using the Agilent Cary 630 FTIR spectrometer. The picture-driven software also reduces training needs and minimizes the risk of user-based errors.

Results and discussion

The binder samples were analyzed by placing a small quantity of solid material directly onto the ATR crystal of the Cary 630 FTIR spectrometer. Gentle pressure was applied to ensure good contact. After the measurement was completed, the ATR crystal was cleaned with a light solvent and wipe in preparation for the next sample.

The MicroLab software uses a built-in Similarity algorithm that automatically calculates a Hit Quality Index (HQI). The HQI value indicates how closely the acquired sample spectrum matches a reference spectrum from the user-generated library. HQI values are commonly used as pass/fail criteria in material identification and confirmation workflows.

Using the Similarity algorithm, all four unknown samples (samples 1 to 4) were correctly identified according to the binder type stated on the respective container labels. However, variations in HQI values were observed among the PVDF samples (1 to 3). As shown in Table 2, PVDF-210 and PVDF-5130 exhibited HQI values of 0.96271 and 0.96713, respectively, indicating strong spectral matches. PVDF-6020 showed a slightly lower HQI of 0.90741, which may reflect differences in polymer grade or formulation compared to the reference sample. PTFE-104 (Sample 4) was also correctly identified, with a high HQI of 0.98345, suggesting good spectral agreement and a high-confidence match.

Table 2. Binder identification results obtained using the Agilent Cary 630 FTIR with ATR and Similarity search algorithm.

"Unknown" Sample	Sample Name	Material Identification	Hit Quality Index
1	PVDF-210	Poly(vinylidene fluoride)	0.96271
2	PVDF-5130	Poly(vinylidene fluoride)	0.96713
3	PVDF-6020	Poly(vinylidene fluoride)	0.90741
4	PTFE-104	Poly(tetrafluoroethylene)	0.98345

The Cary 630 FTIR simplifies result interpretation by displaying color-coded confidence indicators based on user-defined HQI thresholds (Figure 4). In this study, HQI values above 0.95 were color-coded in green, indicating a good spectral match and providing a high level of confidence in the identification of the material for those samples. This visual feedback, combined with fully automated library searching and results display, transforms the Cary 630 FTIR into a turnkey solution for fast, reliable material identification. From sample placement to final result, the MicroLab software minimizes the need for user interpretation, reduces the risk of error, and supports fast decision-making on the production floor.

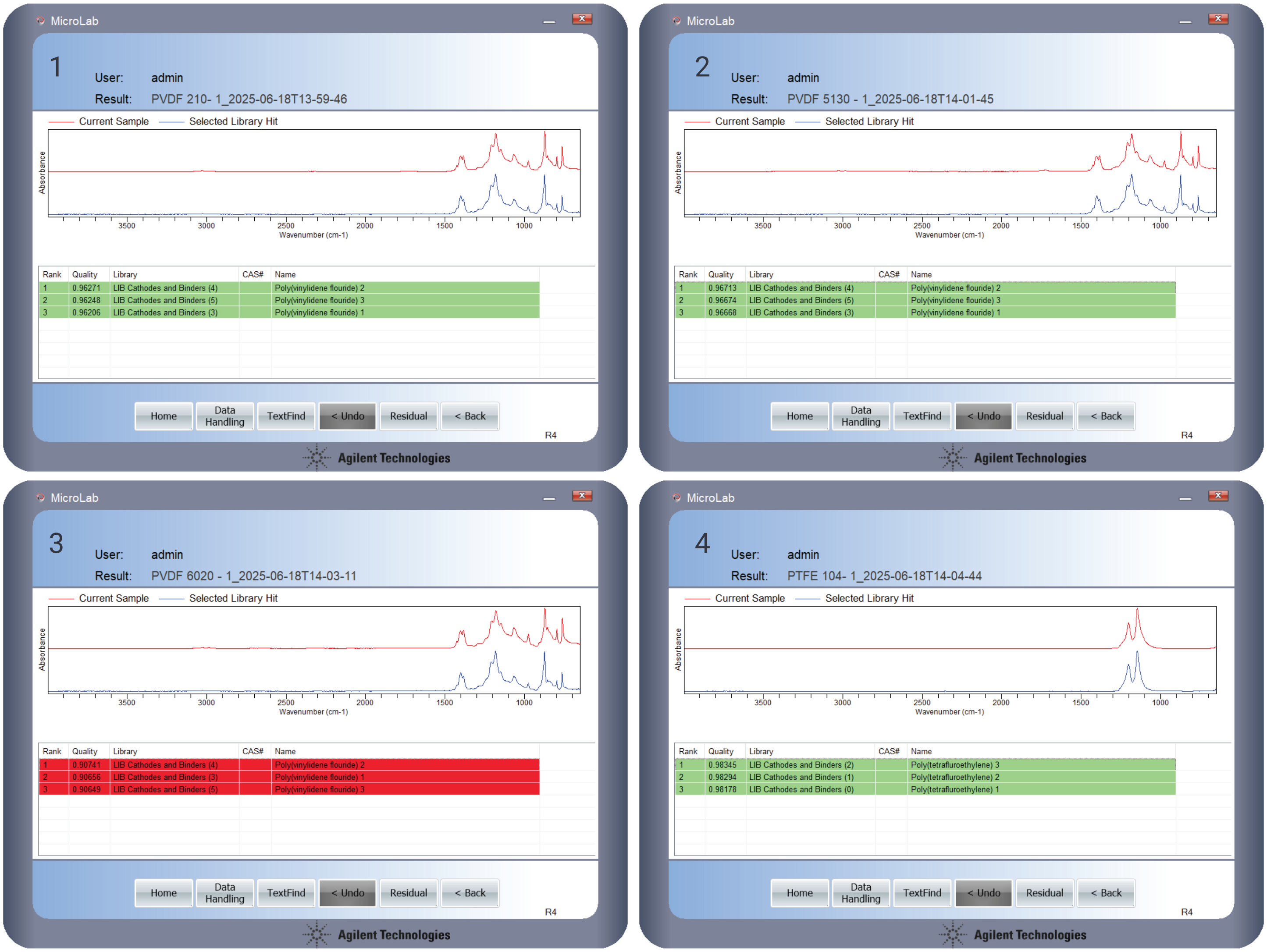

Figure 4. Identification results for the four LIB binder samples using an Agilent Cary 630 FTIR spectrometer. The red traces represent the measured spectra of the unknown samples, while the blue traces show the corresponding library matches. The accompanying tables show the hit quality index (HQI), the reference library used, and the identified material for each sample.

Characterization of PVDF polymorphic phases

FTIR spectroscopy is a valuable tool for distinguishing the crystalline phases of PVDF, which primarily exists in α, β, and γ polymorphic forms. Each phase exhibits distinct IR absorption bands due to differences in molecular conformation:[1]

- The nonpolar α-phase, typically formed through melt processing, is identified by peaks at 763, 795, 855, 976, and 1,149 cm^{-1} and is considered the most thermodynamically stable.
- The β-phase, known for its strong piezoelectric and ferroelectric properties, displays characteristic peaks at 840, 1,275, and 510 cm^{-1}, making it ideal for applications in sensors and actuators.
- The γ-phase, which has intermediate characteristics, is observed with peaks near 812 and 1,234 cm^{-1} and can be induced through specific treatments such as stretching or annealing.

As shown in Figure 5, the three unknown PVDF samples analyzed by the Cary 630 FTIR showed IR absorption peaks corresponding to the α-phase, confirming their nonpolar nature. FTIR's sensitivity to these unique vibrational signatures makes it indispensable for QC testing. It is also useful for the development of new materials, including binders, enabling researchers and manufacturers to tailor properties for enhanced performance in advanced technologies.

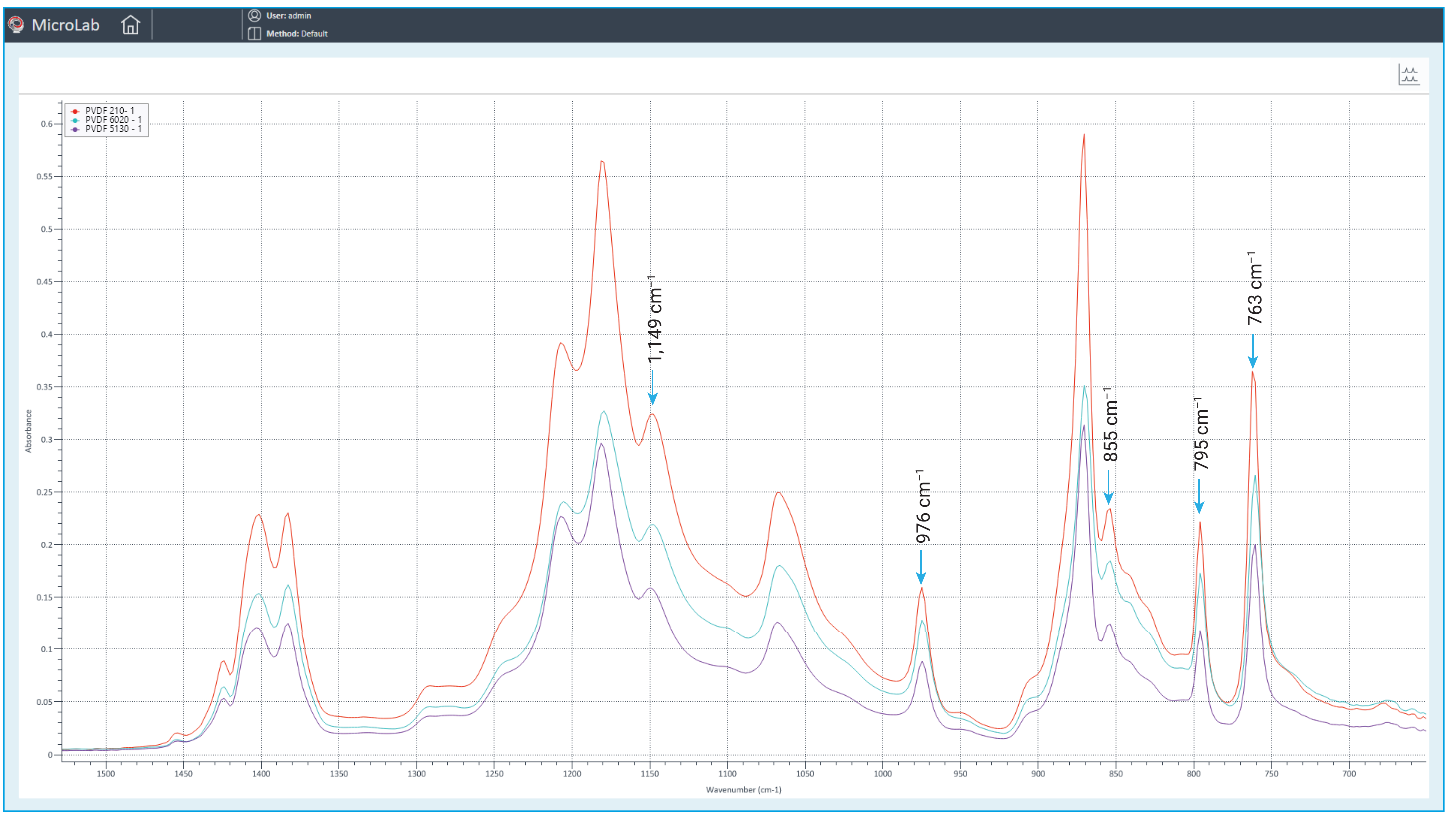

Figure 5. Overlay of three PVDF samples analyzed by an Agilent Cary 630 FTIR, showing peaks corresponding to α-phase IR absorption.

Conclusion

An Agilent Cary 630 FTIR spectrometer with Agilent MicroLab software provided a simple solution for identifying electrode binder materials—a typical application in lithium-ion battery quality control (QC) workflows.

The MicroLab software enabled the rapid creation of a spectral reference library for binder materials based on the analysis of two known "reference" samples. Four "unknown" binders from a different supplier were then correctly identified using the FTIR method. However, one sample yielded a low, red color-coded confidence score, suggesting possible differences in polymer grade or formulation between the reference and unknown samples.

The Cary 630 FTIR enables production and QC teams to:

- Adapt quickly to new materials or suppliers through easy management of the spectral library
- Verify the identity of incoming raw materials using intuitive pictorial guidance and color-coded pass/fail results
- Detect any mislabeling or contamination of materials
- Monitor batch-to-batch variability that could affect electrode performance and battery manufacturing yields

With its compact, modular design, the Cary 630 FTIR can be deployed in production environments, including gloveboxes. Its ease-of-use makes it a valuable tool for ensuring material consistency, minimizing process disruptions, and maintaining high standards in lithium-ion battery manufacturing.

Reference

1. Cai, X.; Lei, T.; Sun, D.; Lin, L. A Critical Analysis of the α, β and γ Phases in Poly(Vinylidene Fluoride) using FTIR. *RSC Advances* **2017**, *7(25)*, 15382–15389.

Further information

- Agilent Cary 630 FTIR Spectrometer
- MicroLab FTIR Software
- MicroLab Expert
- FTIR Analysis & Applications Guide
- FTIR Spectroscopy Basics – FAQs
- ATR-FTIR Spectroscopy Overview

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