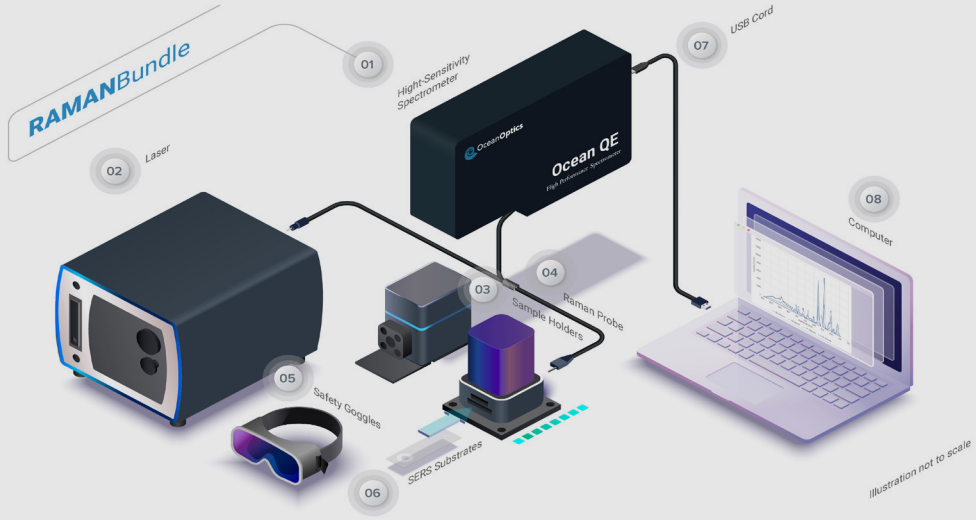
Qualifying the Performance of the QE *Pro*-Raman+ Spectrometer

Application Note



KEYWORDS

- Back-thinned CCD array spectrometer
- Sensitivity
- Organic solvents

TECHNIQUES

- Raman spectroscopy
- Surface Enhanced Raman Spectroscopy (SERS)

APPLICATIONS

- Solvents measurement
- Pesticide detection
- Trace level analysis

Modular spectrometer systems allow for great flexibility in benchtop laboratory measurement, and can be configured into setups ideal for integration into process lines.

One such instrument family is the Ocean Optics QE *Pro* spectrometer platform. The QE *Pro* is a back-thinned CCD array spectrometer that meets the signal to noise, dynamic range and sensitivity criteria necessary for Raman and low light level applications.

To demonstrate key performance improvements in the QE *Pro*-Raman+, we compared it with a similar back-thinned CCD array spectrometer over a series of Raman measurements.

Equipment Used

Our modular Raman setup **(Figure 1)** comprised the QE *Pro*-Raman+ spectrometer, 785 nm Raman excitation laser and safety goggles, Raman probe and sample holder, and spectroscopy software. Variations of this setup are readily available.

Figure 1. Illustration of component parts of modular Raman equipment. SERS substrates can be integrated into systems like this to further enhance sensitivity.

US +1 727-733-2447
EUROPE +31 26-3190500
ASIA +86 21-6295-6600

info@oceanoptics.com • **www.oceanoptics.com**

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Measurement Set 1

To demonstrate the enhanced sensitivity of the QE *Pro*-Raman+, we measured a series of organic solvents. Organic solvents typically have strong and repeatable Raman scattering characteristics, so they work very well as standards against which to compare system performance.

Measurements were performed in OceanView spectroscopy software, applying a 1 second integration time and a single scan to average. The software's "CleanPeaks" function was applied to flatten the baseline of the resulting spectra. Clean- Peaks is a built-in algorithm that can be applied to raw Raman spectra to remove the baseline and any fluorescence.

The results for acetone, isopropanol and methanol are shown in **Figures 2-4**.

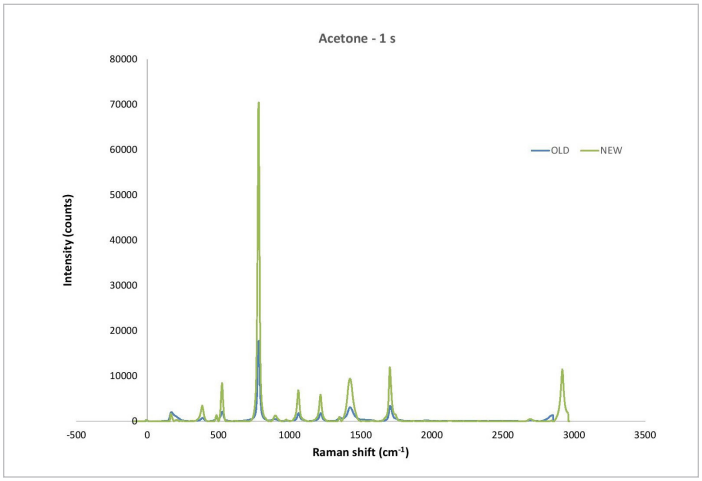

Figure 2. Comparison between an older-model back-thinned CCD array spectrom- eter and the QE *Pro*-Raman+ for acetone at a 1 second integration time.

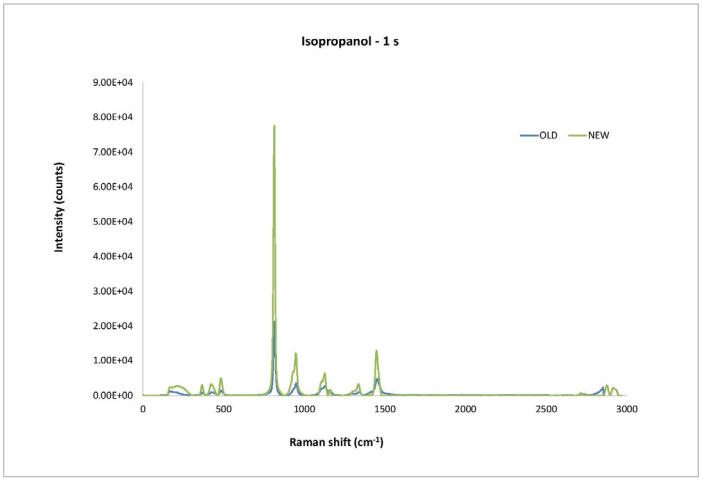

Figure 3. In measurements of isopropanol, the increased sensitivity of the QE *Pro*-Raman+ is evident.

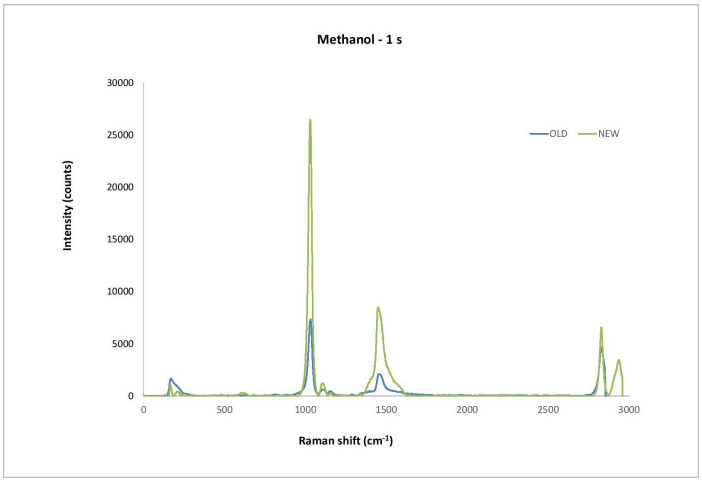

Figure 4. The range of the QE *Pro*-Raman+ is advantageous when measuring samples such as methanol, which has strong peaks around 3000 cm-1.

Measurement Set 2

For our next set of measurements, we took 6 QE *Pro*-Raman+ spectrometers and measured a sample of cyclohexane, with all other system components remaining the same. The integration time in every case was 1 second. This provided insight into the range of sensitivities that can be expected across multiple instruments.

While not all spectrometers were identical in performance, the quality of results was highly consistent **(Figure 5)**. This consistency suggests the spectrometer will work well for quality control and similar applications where repeatability is vital.

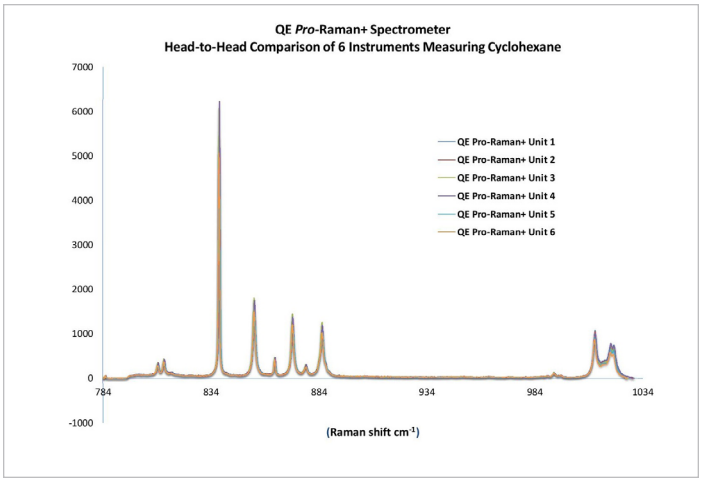

Figure 5. As these series of measurements demonstrate, the QE *Pro*-Raman+ offers a high degree of unit-to-unit consistency.

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Measurement Set 3

Modular, back-thinned CCD array spectrometers like the QE *Pro*-Raman+ are also well suited to surface-enhanced Raman spectroscopy, which allows very low levels of analyte to be detected using colloidal nanoparticles. To test this, we used a SERS gold nanoparticle colloid to detect trace amounts of the fungicide thiram.

Initially, we added 40 uL of 1 ppm thiram to 1 mL liquid SERS. This concentration was determined as relevant from tolerances established by the U.S. Code of Federal Regulations for residues of the fungicide thiram (tetramethyl thiuram disulfide) in or on raw agricultural commodities as follows:

COMMODITY	PARTS PER MILLION
Apple	7.0
Banana	0.8
Peach	7.0
Strawberry	7.0

Source: Federal Register, Thiram; Pesticide Tolerance, A Rule by the Environmental Protection Agency on 09/23/2009 (federalregister.gov)

The resulting SERS spectra **(Figure 6)** clearly demonstrated that thiram at 1 ppm concentration was well within regulatory detection limits for both spectrometers, with even more dramatic results with the QE *Pro*-Raman+ spectrometer

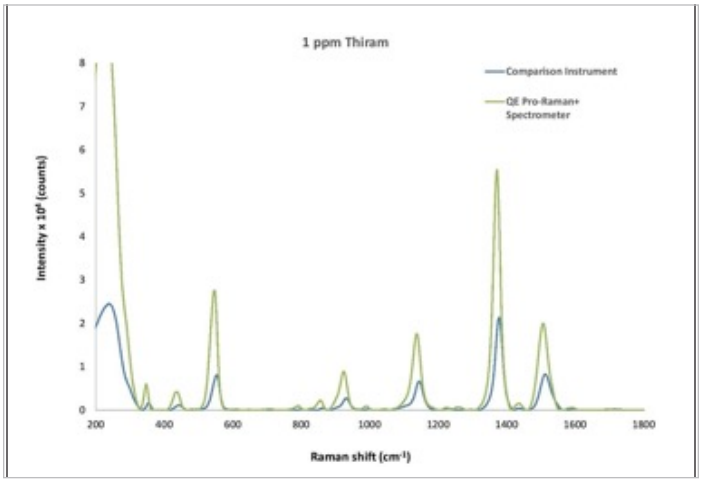

Figure 6. After adding SERS gold nanoparticles to a thiram measurement setup, the sensitivity improvement with QE *Pro*-Raman+ is even more pronounced.

Summary

Increased sensitivity relative to comparable back-thinned CCD array spectrometers was clearly and consistently demonstrated in the QE *Pro*-Raman+. The importance of increased sensitivity is evident in limits of detection studies, since the signal will remain detectable over the noise floor at ever diminished concentrations.