High Resolution Full Range **Ultraviolet** Raman Spectrograph

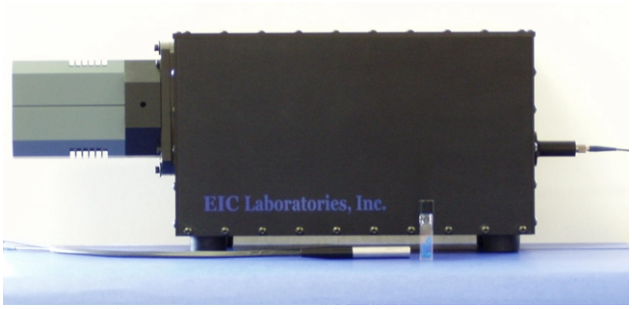
Introduction

Raman spectroscopy provides highly specific information about chemicals of relevance in the fields of medicine, process analyses, and homeland defense. Normal Raman spectroscopy suffers from low sensitivity due to the inherent weakness of the technique. To evaluate samples where the analyte is in trace (ppm or lower) concentrations, enhanced Raman techniques, such as Surface-Enhanced Raman Spectroscopy (SERS) or Resonance Raman Spectroscopy (RRS) are needed. SERS can provide very good sensitivity, but requires adsorption to a metal substrate. For noninvasive measurements, RRS is preferred. In RRS, the laser excitation wavelength overlaps an electronic transition of the analyte of interest. This overlap leads to enhanced Raman signals for the vibrations associated with that electronic transition. RRS simultaneously provides increased sensitivity and selectivity for the analyte of interest. As examples of relevance, RRS has been used to study protein dynamics at biochemically relevant concentrations and to monitor drug intercalation into DNA.

One of the major obstacles to routine usage of RRS is that the electronic transitions of most molecules of interest are in the ultraviolet (UV) wavelength range. The nonlinear relationship between wavelength and frequency has forced tradeoffs in the application of UVRRS. To achieve a reasonable level of resolution, a long path (1 m) double or triple spectrograph was required that is costly, takes significant space, weighs over 100 lbs., has poor throughput, and yields only a limited range in a spectral scan. In contrast, a more compact system could be used with poor (> 20 cm^{-1}) resolution, but range restrictions would still exist.

The EIC vERA Spectrograph

To overcome current limits to the technique and allow UVRRS to become a practical option for laboratory and field investigators, EIC Laboratories has developed the EIC vERA spectrograph. The spectrograph is based on an echelle grating that enable two-dimensional dispersion of the desired spectrum across the detection element.



The EIC ERA Spectrograph and UV Raman Probe.

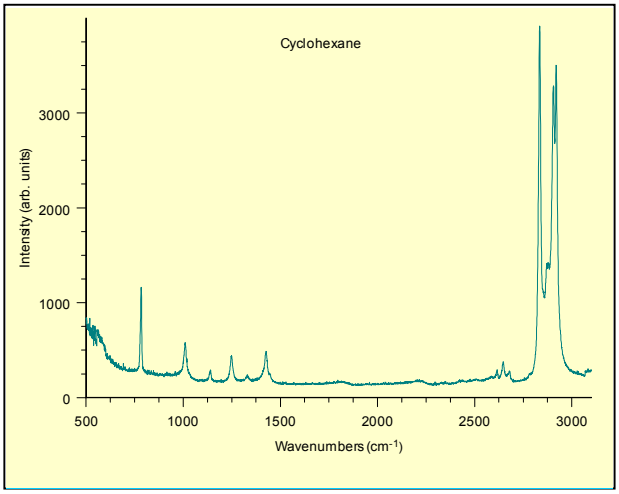
The EIC vERA Spectrograph is portable and can be transported without losing calibration. The system can also use fiber optic Raman probes, such as the ½" diameter head probe sold by our commercial subsidiary, InPhotonics. The implementation enables field, *in situ*, and *in vivo* diagnostics to be performed.

System Specifications

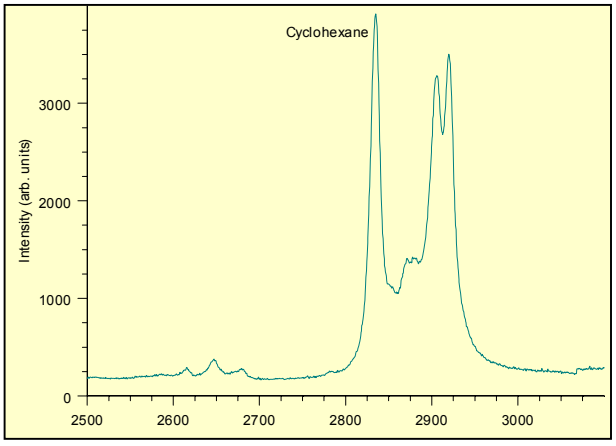
Parameter	Value
Range	200-3500 cm^{-1}
Resolution	6 cm^{-1}
Dimensions:	
Spectrograph	14 ½ " L x 7 ¾ " W x 8 ¼ " H
Detector	6 ¾ " L x 4 ½ " W x 4 " H
Weight	29 lbs.
Electrical Requirements	120 V AC
Ambient Operating conditions	Not to exceed 35°C

Simultaneous Range and Resolution

The EIC νERA collects full spectral range (200-3500 cm^{-1}) at a resolution of 4-6 cm^{-1} in one acquisition. Practically, the filtering requirement restricts the lowest detectable frequencies. With vapor filters, peaks within ±25 cm^{-1} of the laser line have been detected, while standard filters will block the first 600 cm^{-1}. The range and resolution are demonstrated below.



UV Raman spectrum of cyclohexane collected with <500 µW laser power at 248 nm.

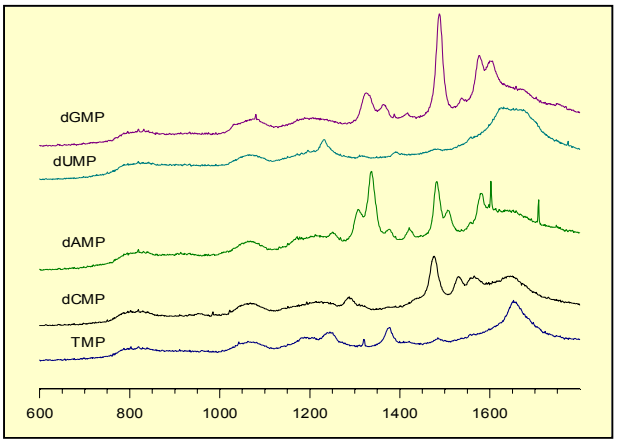


Expansion of the C-H stretching region to demonstrate resolution.

In addition to having greater range, the EIC νERA has superior throughput compared to conventional triple spectrographs. The νERA has throughput very close to the InPhotonics RS2000, a NIR full range Raman spectrometer.

Applications

Homeland Defense – UVRRS can be used for detection of chemical warfare agents as all have electronic transitions in the UV. The military is currently developing a UV lidar system for remote detection of warfare agents. In addition, nucleic acids have electronic transitions around 250 nm. One way to differentiate biological clouds is to detect the DNA. Further, research has shown that the nucleic acid ratio is unique for bacterial species and can be used for taxonomic identification to identify biological agents.[1]



UVRRS of 500 µM concentrations of the common nucleic acids.

Medical – In addition to nucleic acids, UVRRS can be used for protein analysis. Tryptophan peak position and amide features allow precise structural and hydrophobic/hydrophilic information on the protein. Mutations and rare variants of hemoglobin can be detected. UVRRS has been used for colon histochemistry. Determination of virus structures can be performed. Finally, UVRRS can probe the effectiveness of new medications by verifying drug incorporation into tissues, cells, or DNA grooves.

Process Control – UVRRS has been used to monitor plastic degree of polymerization as well as coating quality on materials.

For more information, please contact:

Dr. Kevin Spencer
Director, Spectroscopy Division
spencer@eiclabs.com

[1] E. Ghiamatti, R. Manoharan, W.H. Nelson and J.F. Sperry, Appl. Spectrosc., **46**, 357-64 (1992).