



A Raman Spectroscopic Comparison of Xylene Isomers: *meta*-xylene, *ortho*-xylene and *para*-xylene

Background:

Raman spectroscopic analysis is an ideal method for identifying chemical samples and even distinguishing isomers of the same chemical. Ocean Optics offers many options of ready to use Raman systems with different resolution, sensitivity and laser wavelength options, including a low-resolution hand held device and desktop units.

To illustrate the capabilities of our Raman equipment, we analyzed xylene and its three isomers (*meta*-, *ortho*- and *para*-xylene). Each of these three designations refers to a specific location that the two methyl groups are attached to the benzene ring. Typically these isomers are found in technical grade xylene (mixture) in the proportions of 45-55% *m*-xylene and approximately 20% of each of the *p*- and *o*-xylene, with the remainder consisting of ethylbenzene.

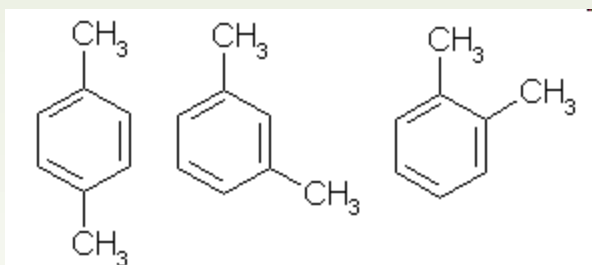


Figure 1. *Para*-, *meta*-, and *ortho*-xylene isomers

Xylene is one of the most widely used chemicals. It is used as a solvent in vast industries, from leather and printing to rubber and plastic. It is also used for cleaning steel, as a paint thinner, and can be found in gasoline and airplane fuel.

Due to its potentially adverse health effects, xylene falls into the volatile aromatic compound (VOC) category. Although xylene is found naturally, it is not usually found at levels of concern in the environment, so, any significant exposures to xylene that occur are the cause of its production and use. Regulatory agencies monitor the levels of xylene in drinking water, in the workplace, and in the environment to protect people from its potential harmful health effects.

Experimental:

The isomers of the aromatic organic compound xylene, *meta*-xylene, *ortho*-xylene, and *para*-xylene, as well as a mixture of all three isomers of xylene, were selected for Raman spectroscopy testing to determine if our equipment can identify each isomer. The first set of measurements were made using a Maya2000 Pro spectrometer (grating H11, 25 μm wide slit, range 530.5-653.0 nm, 0.10 nm FWHM), which has a peak 75% quantum efficiency, SpectraSuite software, probe (RIP-Probe-532) and laser (VD-III A DPSS Laser Driver 532 Laser). All measurements utilized the same acquisition parameters of 11 seconds integration time, 1 scan to average and 0 box cars. Samples of each chemical were prepared and placed in glass vials measuring 5.5 cm tall and 4.7 cm in circumference. The vials were placed separately into a closed sample holder into which the laser probe was directed.



The second set of measurements were made using a QE65000-Raman spectrometer (grating H6, 50 μm wide slit, range 779.4-932.4 nm, optical resolution 0.40 nm FWHM), which has a 90% quantum efficiency, SpectraSuite spectrometer operating software, probe (RIP-Probe-785), and laser (LASER-785-IP). All measurements utilized the same acquisition parameters of 1200 milliseconds integration time, 1 scan to average and 0 box cars. Samples of each chemical alcohol were prepared and placed in glass vials measuring 5.5 cm tall and 4.7 cm in circumference. The vials were placed separately into a closed container into which the laser probe was directed.

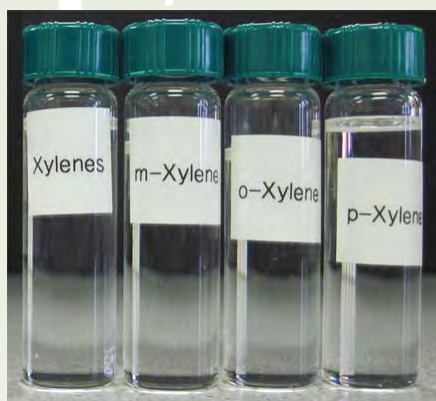


Figure 2. Xylene samples



Figure 3. Equipment set-up: 532-laser, Maya2000 Pro, and probe



Figure 4. Equipment set-up: 785- laser, QE65000, and probe

Results

Comparisons of xylene and its isomers were overlaid using the SpectraSuite software. These overlays were used to identify similar and dissimilar characteristics of xylene and its isomers.

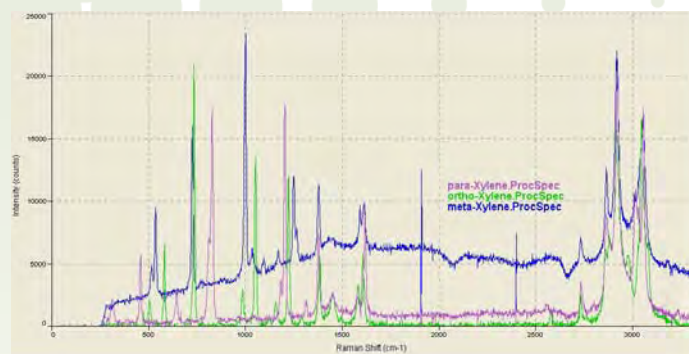


Figure 5. Raman spectra with 532-laser of xylene isomers

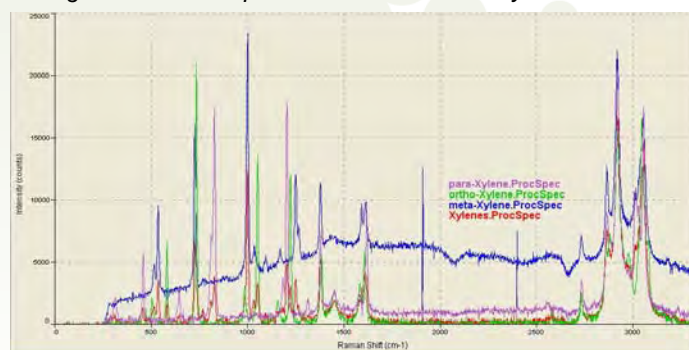


Figure 6. Raman spectra with 532-laser of xylene isomers and technical grade xylene mixture

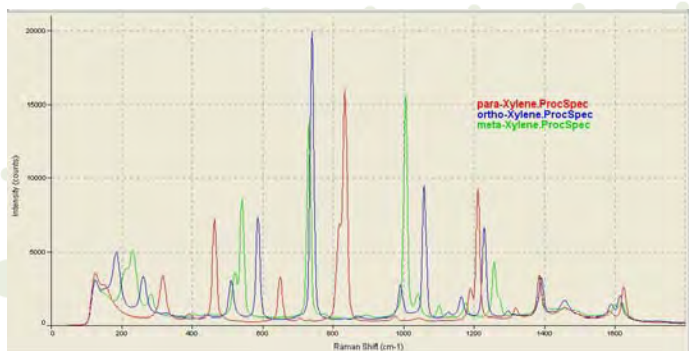


Figure 7. Raman spectra with 785-laser of xylene isomers

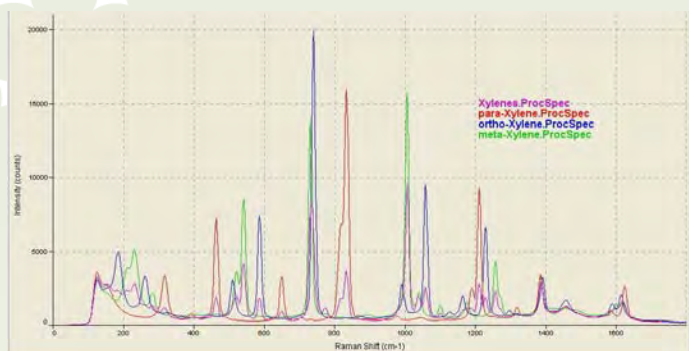


Figure 8. Raman spectra with 785-laser of xylene isomers and technical grade xylene mixture

Conclusions:

Raman spectroscopy can be achieved easily with Ocean Optics equipment. The three isomers of xylene can be distinguished using both 532 and 785 laser excitation.

With 532 excitation, typical fluorescence occurs for meta-Xylene. Some peaks are shared between all three isomers, but there are many differences in peak values that can provide differentiation.

While the measurements with the MAYA2000 Pro could have been improved with more scans to average, the results achieved with the QE65000 are noticeably cleaner spectra due to the nature of the high sensitivity of our scientific grade spectrometer with 90% quantum efficiency and high signal to noise ratio.

Raman spectroscopy is a powerful quantitative and qualitative tool for a wide range of analytical applications, both in the laboratory and in the field.

Related References:

“Coherent mode-selective Raman excitation towards standoff detection,” H. Li, D. Harris, B. Xu, et al. *Optics Express*, 16(8): 1-6 (2008) Retrieved from <http://www2.chemistry.msu.edu/faculty/dantus/publications/pub%20135.pdf>

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“Light at the end of the tunnel: recent analytical applications of liquid-core waveguides,” T. Dallas, P. Dasgupta, *Trends in Analytical Chemistry*, 23(5): 1-8 (2004) Retrieved from www.depts.ttu.edu/ntc/Personnel/Dallas/Dallas_Publication_pdfs/TrAC_04.pdf