



Standard Guide for Relative Intensity Correction of Raman Spectrometers¹

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1. Scope

1.1 This guide is designed to enable the user to correct a Raman spectrometer for its relative spectral-intensity response function using NIST Standard Reference Materials² in the 224X series (currently SRMs 2241, 2242, 2243, 2244, 2245, 2246), or a calibrated irradiance source. This relative intensity correction procedure will enable the intercomparison of Raman spectra acquired from differing instruments, excitation wavelengths, and laboratories.

1.2 The values stated in SI units are to be regarded as standard. No other units of measurement are included in this standard.

1.3 Because of the significant dangers associated with the use of lasers, ANSI Z136.1 or suitable regional standards should be followed in conjunction with this practice.

1.4 *This standard does not purport to address all of the safety concerns, if any, associated with its use. It is the responsibility of the user of this standard to establish appropriate safety and health practices and determine the applicability of regulatory limitations prior to use.*

2. Referenced Documents

2.1 *ASTM Standards:*³

E131 Terminology Relating to Molecular Spectroscopy

E1840 Guide for Raman Shift Standards for Spectrometer Calibration

E2529 Guide for Testing the Resolution of a Raman Spectrometer

2.2 *ANSI Standard:*⁴

Z136.1 Safe Use of Lasers

3. Terminology

3.1 *Definitions*—Terminology used in this practice conforms to the definitions in Terminology E131.

4. Significance and Use

4.1 Generally, Raman spectra measured using grating-based dispersive or Fourier transform Raman spectrometers have not been corrected for the instrumental response (spectral responsivity of the detection system). Raman spectra obtained with different instruments may show significant variations in the measured relative peak intensities of a sample compound. This is mainly as a result of differences in their wavelength-dependent optical transmission and detector efficiencies. These variations can be particularly large when widely different laser excitation wavelengths are used, but can occur when the same laser excitation is used and spectra of the same compound are compared between instruments. This is illustrated in Fig. 1, which shows the uncorrected luminescence spectrum of SRM 2241, acquired upon four different commercially available Raman spectrometers operating with 785 nm laser excitation. Instrumental response variations can also occur on the same instrument after a component change or service work has been performed. Each spectrometer, due to its unique combination of filters, grating, collection optics and detector response, has a very unique spectral response. The spectrometer dependent spectral response will of course also affect the shape of Raman spectra acquired upon these systems. The shape of this response is not to be construed as either “good or bad” but is the result of design considerations by the spectrometer manufacturer. For instance, as shown in Fig. 1, spectral coverage can vary considerably between spectrometer systems. This is typically a deliberate tradeoff in spectrometer design, where spectral coverage is sacrificed for enhanced spectral resolution.

4.2 Variations in spectral peak intensities can be mostly corrected through calibration of the Raman intensity (y) axis.

¹ This guide is under the jurisdiction of ASTM Committee E13 on Molecular Spectroscopy and Separation Science and is the direct responsibility of Subcommittee E13.08 on Raman Spectroscopy.

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² Trademark of and available from NIST Office of Reference Materials, 100 Bureau Drive, Stop 2300, Gaithersburg, MD 20899-2300. <http://www.nist.gov/srm>.

³ For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

⁴ Available from American National Standards Institute (ANSI), 25 W. 43rd St., 4th Floor, New York, NY 10036, <http://www.ansi.org>.