

INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

PHYSICAL CHEMISTRY DIVISION
COMMISSION ON MOLECULAR STRUCTURE
AND SPECTROSCOPY

RECOMMENDATIONS FOR THE
PRESENTATION OF RAMAN
SPECTRA FOR CATALOGING
AND DOCUMENTATION IN
PERMANENT DATA
COLLECTIONS

LONDON
BUTTERWORTHS

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The use of optical lasers as exciting sources has led to increasing use of Raman spectrophotometry in chemical research, and it is desirable that Raman spectra intended for cataloging and documentation in permanent collections should be presented in a uniform manner. Commission 1.5 (Molecular Structure and Spectroscopy) therefore proposes that the following recommendations be followed. These have been prepared after consultation with many spectroscopists concerned with the documentation of Raman spectral data.

There is agreement that various quality levels of documented Raman spectra are needed. Suggested possibilities for liquid state systems are:

(a) A collection of Raman spectra determined by standard methods meeting the recommendations noted below, with a separate tabulated listing of the depolarization factors.

(b) A collection similar to (a) but with a presentation of the infrared spectrum on the same chart above the Raman spectrum with the same abscissa.

(c) Raman spectra presented with curves for different polarizations.

(d) Raman spectra recorded digitally and subsequently computer corrected for instrumental factors. Among these correction factors are (i) photo-detector response; (ii) grating blaze. Such spectra may appropriately be recorded as separate plots of the depolarization factors $(\alpha')^2$ and $(\gamma')^2$.

For crystalline powder spectra the formats (a) and (b) are appropriate.

RECOMMENDATIONS

(1) Spectra should be recorded or presented so as to make them compatible with, and suitable for comparison along side of, recorded infrared spectra. A 2:1 scale compression is desirable above 2000 cm^{-1} as is customary with recorded infrared spectra. The ordinate scale should be linear intensity measured upwards and the abscissal scale linear $\Delta\nu\text{ (cm}^{-1}\text{)}$, decreasing left to right. Chart paper should preferably be marked in the metric system (e.g. cm^{-1}/cm).

(2) The intensity may be adjusted to be off scale by a factor not exceeding

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1000 if this is necessary to obtain a satisfactory record of the weaker significant bands. The strongest bands should then be rescanned at an appropriately reduced intensity with the intensity reduction ratio indicated in the chart.

(3) Corrections for instrumental response should be indicated. A desirable practice would be the presentation of the instrumental response to a standard lamp for all necessary polarization orientations. This may take the form of a curve or may be tabulated. If computer or digital readout is available, it is recommended that the standard lamp corrections be applied to the spectral data. This should be indicated on the chart.

(4) The following operational parameters should be specified:

(a) The spectral slit width (cm^{-1}) should be given at several places in the spectrum.

(b) The wavelength or wavenumber of the exciting radiation and the nominal power of this radiation measured at the sample location. (Include the approximate number of reflections in a multipass cell.)

(c) The spectral scanning rate and period, i.e. 4 times the instrumental time constant.

(d) The type of spectrometer and detecting system used.

(e) The geometry of the sample excitation, including the polarization geometry. Porto's $x(yy)z$ notation is acceptable with specified axes.

(f) The physical state of the sample including as much quantitative information as possible concerning concentration, temperature, and pressure where such data are relevant.

(5) Depolarization factors. The following alternatives are appropriate for liquid and gas or vapor samples:

(a) A list of ρ values for the spectrum of each substance, submitted as a separate set of tabulated data.

(b) A graphical record of the spectrum measured in the two necessary polarization orientations. These may be on separate charts or superimposed.

(c) For data recorded digitally, graphical records on one or separate charts for the two polarizability components $(\alpha')^2$ and $(\gamma')^2$.