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General rules for Raman spectrometry

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Foreword

This translation has been made based on the original Japanese Industrial Standard established by the Minister of Economy, Trade and Industry through deliberations at the Japanese Industrial Standards Committee according to the proposal for establishment of Japanese Industrial Standard submitted by Japan Analytical Instruments Manufacturers' Association (JAIMA)/Japanese Standards Association (JSA) with the draft being attached, based on the provision of Article 12 Clause 1 of the Industrial Standardization Law.

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General rules for Raman spectrometry

1 Scope

This Japanese Industrial Standard specifies general rules for Raman spectrometry where Raman scattering spectrum of substance is measured by using Raman spectrometer according to the excitation light in the region from ultraviolet and visible to near infrared, then the qualitative analysis and the quantitative analysis of substance are carried out.

2 Normative references

The following standards contain provisions which, through reference in this text, constitute provisions of this Standard. The most recent editions of the standards (including amendments) indicated below shall be applied.

JIS C 6802 *Safety of laser products*

JIS K 0050 *General rules for chemical analysis*

JIS K 0211 *Technical terms for analytical chemistry (General part)*

JIS K 0212 *Technical terms for analytical chemistry (optical part)*

JIS K 0215 *Technical terms for analytical chemistry (Analytical instrument part)*

3 Terms and definitions

For the purposes of this Standard, the terms and definitions given in JIS K 0050, JIS K 0211, JIS K 0212 and JIS K 0215, and the following apply.

3.1 Raman shift

a difference in wave number between excitation light and Raman scattering light

It is expressed by the frequency, difference in vibration number and difference in energy corresponding to the molecular vibration.

3.2 linear Raman scattering, spontaneous Raman scattering

Raman scattering having the intensity proportional to the intensity of incident light

It is used to distinguish it from the non-linear Raman scattering by the higher order non-linear optical effect.

3.3 Stokes Raman scattering

Raman scattering shifting from the wave length, wave number, number of vibration or frequency, or energy of the incident excitation light to the long wave length, low wave number, low number of vibration or low frequency, or low energy side

3.4 anti-Stokes Raman scattering

Raman scattering shifting from the wave length, wave number, number of vibration or

frequency, or energy of the incident excitation light to the short wave length, high wave number, high number of vibration or high frequency, or high energy side

3.5 vibrational Raman scattering

Raman scattering generated by the vibration transition of molecule

3.6 rotational Raman scattering

Raman scattering generated by the rotational transition of molecule

3.7 electronic Raman scattering

Raman scattering generated by the electronic transition of molecule

3.8 resonance Raman scattering

the phenomenon in which Raman scattering intensity is increased by excitation at the wave length being close to the electronic absorption of the sample molecule

3.9 Raman scattering circular dichroism, Raman optical activity

the phenomenon in which Raman scattering intensity differs between the left-circularly polarized light and the right-circularly polarized light

3.10 depolarization ratio

the intensity ratio of the polarization component of Raman scattering vertical to the polarization plane of incident laser light to the polarization component of Raman scattering parallel to it

3.11 nonlinear Raman scattering

Raman scattering having the intensity proportional to the second order or higher of intensity of incident light

It is used to distinguish it from the linear (spontaneous) Raman scattering.

3.12 surface enhanced Raman scattering

the significantly enhanced Raman scattering observed for molecules adsorbed on metal surface or metal colloid

3.13 half-wave plate

the phase plate to change the difference of optical path of orthogonal vibrating polarizations by $1/2$ wave length

4 Summary

4.1 Raman scattering

Raman scattering is the non-elastic scattering of the light generated when the energy difference among multiple photons having different energies is equal to the energy difference among the energy levels of substance, and includes not only linear Raman scattering discovered by C.V. Raman but the non-linear Raman scattering. Raman scattering in a limited sense means the linear Raman scattering. In this Standard, Raman scattering is used in a sense of the linear Raman scattering. Raman scattering

has the two components such as Stokes Raman scattering and anti-Stokes Raman scattering and usually means the vibrational Raman scattering; however, it also includes the rotational Raman scattering and the electronic Raman scattering. Usually, Raman shift takes a positive value to the Stokes side and a negative value to the anti-Stokes side.

4.2 Raman spectrum

The graph, in which the ordinate is made to be Raman scattering intensity and the abscissa is made to be Raman shift, is called Raman scattering spectrum (abbreviation: Raman spectrum), and usually indicates only the Stokes Raman scattering. In Raman spectrum, Raman scattering intensity is indicated in optional scale on the ordinate and the abscissa is graduated in Raman shift (cm^{-1}) as the standard; however, Raman shift (Hz), Raman shift (eV), wave number shift (cm^{-1}), number of vibration or frequency shift (Hz), energy shift (eV), wave number (cm^{-1}), number of vibration or frequency (Hz), or energy (eV) are used in same cases. Raman spectrum of indene is shown in figure 1.

NOTE: Care shall be taken so that the indication in which the indicating physical quantity does not correspond to the unit such as energy (cm^{-1}) is not used.

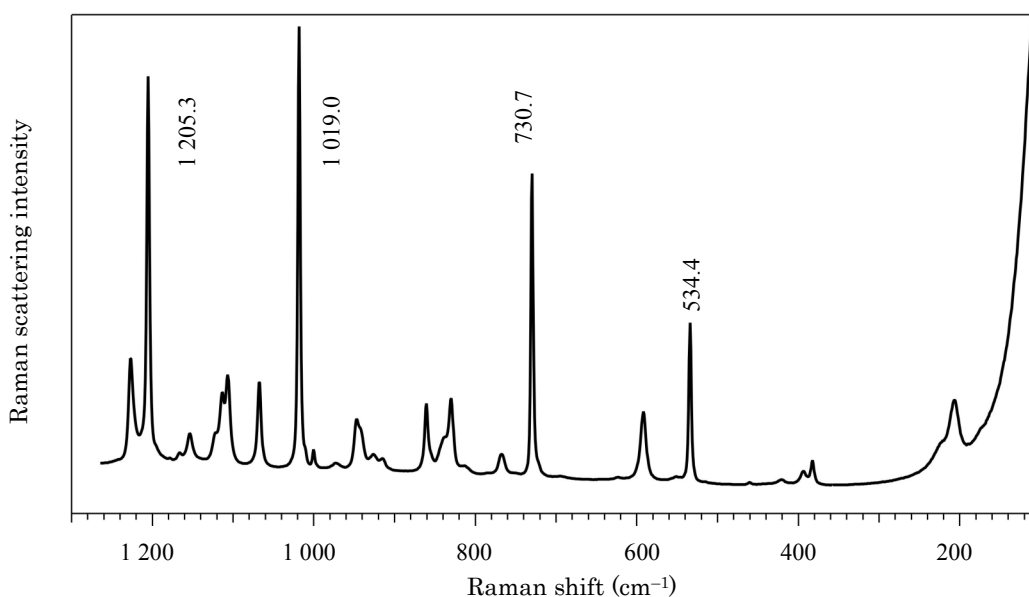


Figure 1 Raman spectrum of indene

4.3 Raman image

The image in which Raman scattering intensities are plotted in two dimensions or three dimensions to the measuring position is called Raman image. Raman image is obtained by the mapping measurement in which the image is created by measuring Raman spectrum from each point of the sample individually or by the direct Raman image measurement in which the image is directly obtained by irradiating excitation light to the whole of sample and filtering Raman scattering light (see figure 2).

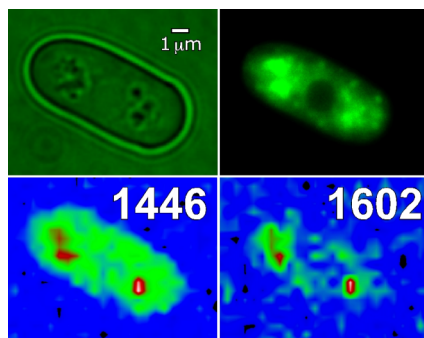


Figure 2 Microscopic image (upper left), green fluorescent image (upper right), Raman image (Raman shift 1 446 cm^{-1}) and Raman image (Raman shift 1 602 cm^{-1}) of fission yeast single live cell

4.4 Characteristics of Raman spectrometry

The characteristics of Raman spectrometry are as follows.

- a) Raman spectrum, as it is called the "fingerprint of molecule", is sensitive to the structure, dynamics or environment of molecule species in the substance, therefore it is suitable for the qualitative analysis, the quantitative analysis or the state analysis of molecule species.
- b) Regardless of the material phase such as gas, liquid, solid, the sample form such as crystal, fibre, film and the environment such as temperature, pressure, it is capable of measuring the sample under the state as it is.
- c) It is capable of measuring the temperature, stress, density, crystallization degree, orientation degree, etc. "on the spot" (*in situ*).
- d) It has a high resolution of time (picosecond). The dynamic analysis of the system changing at high speed is possible.
- e) It has a high resolution of space (sub-micrometer). The local analysis by the space resolution of sub-micrometer, and the imaging analysis by mapping or direct imaging method are possible.
- f) The state analysis by using polarization is possible. The polarization measurement of single crystal, the analysis of molecule symmetry by the measurement of depolarization ratio of liquid or solution, and the analysis of optical activity by the measurement of Raman scattering circular dichroism are possible.
- g) The high sensitivity and selective analysis of molecule species by resonance Raman scattering is possible.
- h) The high sensitivity analysis of surface adsorption species by the surface enhanced Raman scattering is possible.
- i) There are some cases subjected to the strong disturbance due to the fluorescence emitted from the sample itself or foreign matters.
- j) There is a possibility that the sample is damaged by the laser light used for the ex-

citation.

- k) It is not suitable to the trace component analysis (except the resonance Raman scattering and the surface enhanced Raman scattering).

5 Apparatus

5.1 Constitution of apparatus

An example of the constitution of Raman spectrophotometer is shown in figure 3. Raman spectrophotometer shall consist of a light source part, a sample part, a spectral part, a detection part, a data processing part and a display/record/output part. The concept diagram of Raman spectrophotometer is shown in figure 4.

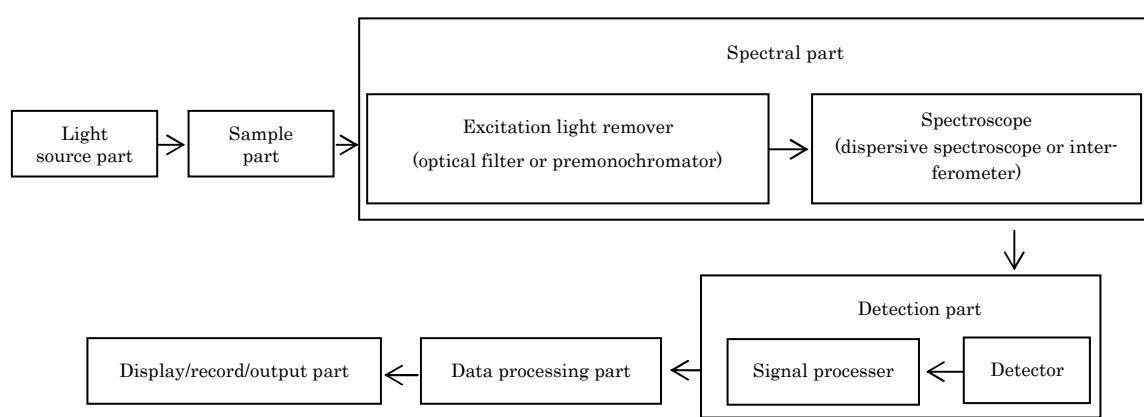


Figure 3 Example of constitution of Raman spectrophotometer