SPECTROSCOPY AND ITS APPLICATION IN GEMMOLOGY

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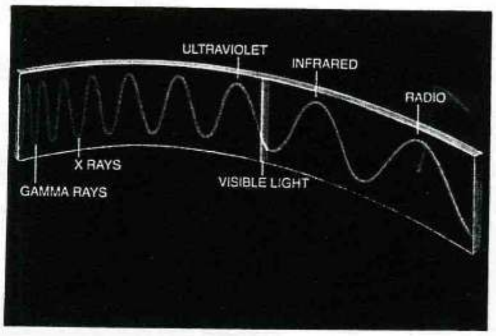
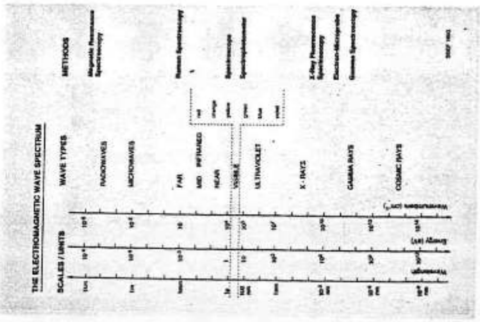
Electromagnetic spectrum (light and other radiation energy)



The fundamentally continuous succession of wavelengths or energies in a rainbow colour band is the most well known spectrum, called the visible spectrum of light. Light is a form of energy that is just a small part of the spectrum of electromagnetic waves. This continuous spectrum consists of light waves from short to increasingly longer wavelengths or energies. An evenly balanced mixture of spectral colour creates white. Each spectral colour or pure colour is termed a spectral hue, e.g. "red". It may also be expressed in terms of wavelengths in nanometres, in terms of energy in eV or wavenumber or frequency. The units are convertible. The vibration of red at 750 (nm) nanometers is equivalent to 13,300 (cm-1) vibrations per cm, with an energy of 1.8 (eV) electron volts. Below the shortest visible rays of violet the spectrum merges into the invisible ultraviolet with higher energies and shorter wavelengths. Beyond the last visible red the spectrum proceeds to infrared which has longer waves and smaller energies respectively, see table 1.



When a gemstone is bathed in light or excited by the energy of incoming waves or radiation, different reactions can take place. Some of the most important characteristics of spectroscopy are absorption (a transformation into other energy forms) and fluorescence (a transformation into electromagnetic waves with lower energy).

In the visible part of the spectrum, any disturbance of the evenly balanced mixture of spectral colours (by absorption or fluorescence) creates a colour other than white or colourless, respectively.

Excitation ("light source")

A device that investigates a definite spectral region must not only record the radiation or energy, but also create the specific spectral force by a "lamp" comparable with the light source in the spectroscope. This could be an X-ray tube for the very short wave X-ray spectrum, a tungsten lamp for the visible, or a glowing ceramic rod for the infrared. Each of those energy sources is "shedding light" on a specific spectral part, see table 2.

An energy source may produce electromagnetic radiation which covers a larger spectral area, i.e. a continuation from longer to shorter waves. In the visible, such a spectrum is called continuous spectrum, or white light.

On the other hand, an excitation or light source may be of one energy or light colour only. It is then called monochromatic. A beam of accelerated electrons can also furnish the energy necessary to study spectroscopic phenomena. Such an electron beam is very similar to a monochromatic source of radiation and is used e.g. in scanning electron microscopes (SEM) as a "light source."

Sample

We usually put our sample or gemstone between the "light source" and the observer, thus the gemstone acts as a selective filter. From the wide spectral supply some portions are consumed by the sample when the light travels through the material or interacts when it hits the surface. From the initially homogeneous distribution of the incoming energy spectrum (or light), a selective absorption or fluorescence may take place and locally put positive or negative intensities into the spectrum.

Dispersing medium ("prism")

Light and other radiation usually include rays of various wavelengths or energies (white light, continuum). For example, sunlight contains all spectral colours. By means of a prism or diffraction grating it is possible to fan the white light to a rainbow colour band. In this way the colour components are individually visible and their relative intensities are measurable. The dispersing medium in this case is the prism or the grating. In other spectral sections it is similarly important to separate the energies when individual behaviour of distinct energies to be studied or recorded. A multichannel analyser may do this job in the X-ray part. An interferrogram setup may do it in an FT- infrared spectrophotometer.

Detector (spectrometer)

In the visible spectral section we register or perceive light with our eyes. Spectroscopes and spectrophotometers are able to show us in detail colour phenomena and also record the observations. In pursuing shorter wave spectral regions like UV, X-rays or gamma rays, we need specially designed instruments to record the characteristics of those waves or energies, respectively. The instruments applied in that spectral part are special detectors or multichannel analyzers. Also for the infrared and radio waves we can register phenomena only with the help of instruments sensitive in those spectral parts.

Display

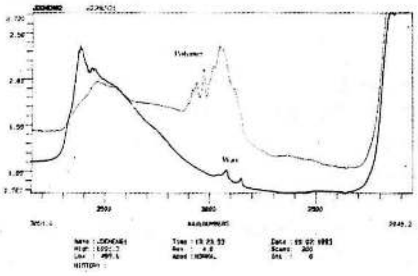
The spectral information usually is displayed in an x/y diagram, where we can see the relative intensities along the selected spectral section. X-axis is used for wavelength (or energy) and y-axis is used for intensity of a distinct wavelength. For example in an emerald absorption spectrum the green of 500 nm is fully transmitted whereas red of 650 nm is strongly absorbed (extraordinary ray). We know that these spectral features are due to the trace element chromium. The curve can be displayed on a printer/plotter, TV-screen, as a curve or in figures.

ectral areas (different evidences)

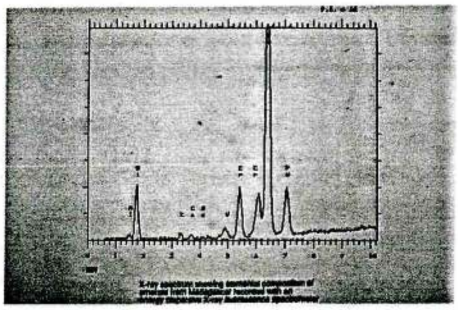
Absorption and fluorescence phenomena in the visible area are produced in many minerals by trace elements responsible for the colour of that individual gemstone.

Examples of spectrograms

1. **Infrared spectrum** of jadeite, and epoxy treated jadeite **(B-jade)**. The spectra in the mid-infrared, recorded with a Fourier transform instrument show molecular absorptions between 2800 and 3200 cm-1 which can be attributed to organic substances. Wax peaks are below 3000 and epoxy-resin peaks are below and **above** 3000 cm-1.



2. **X-ray fluorescence spectrum**, produced by an emerald from Madagascar after excitation by the X-ray radiation of the rhodium tube. The fluorescence energies are plotted and labeled according to the elements which have caused them. The selected filter and tube voltage favours the trace elements vanadium, chrome, iron. For silicium and aluminium the instrument is not so sensitive with the selected conditions. **Trace element** investigation is helpful for a detailed characterisation of natural or synthetic crystals.



It is the energy consumption of valence electrons of the outermost shell which is donated by the energy now missing in the absorption spectrum (= absorption). But there are other causes of colour which are not related to chemical impurities.

The transitions between different energy levels of electrons (from inner shells) can be observed in the X-ray spectral part. If atoms are excited with energy, electrons may jump to higher levels and subsequently fall back to the ground state. This means energy emission which can be recorded and assigned to a definite electron transition in a definite element. Since each element possesses its characteristic electronic architecture the x-ray spectroscopy is a method of determining chemical composition. The spectra are fluorescence line spectra (see diagram "X-ray fluorescence"). A chemical analysis can be done by investigation of the X-ray spectrum.

Bonding energies keep groups of atoms together. Molecules, as they are called, possess a certain freedom to move even when locked in a crystal structure. Atomic groups may swing, rotate or vibrate within certain limits. Molecular vibrational energies possess values within the infrared spectrum. Therefore distinct energies of the supply of an infrared source may satisfy the demand of molecules available to vibrate. This will lead to absorption features in the infrared spectrum.

Conclusions

In many respects, spectroscopy is a matter of supply and demand. Electrons or molecules have a strong tendency to move. The expenses of such movements are paid by taking the necessary energy out of the supplying excitation ("light source"). The result is absorption (or fluorescence) and we can read a spectrogram like an invoice for consumption. In the case of fluorescence the accepted energy is too high, and the balance is rendered like a bonus as fluorescent energy. This general principle is valid for all spectral areas.

Schematic setup of a spectrophotometer

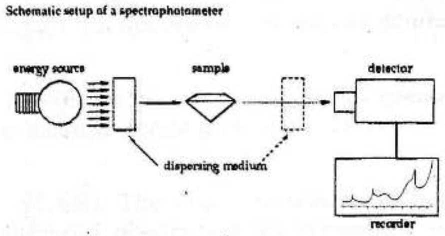


Table 2

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