METHOD OF INTERPRETING SPECTROMETRIC DATA

This application claims benefit of Provisional Application 60/046,944 filed May 19, 1997.

FIELD OF INVENTION

This invention relates generally to light-spectrum-measurements and more specifically to a method of enhancing spectral resolution of an imaged spectrum.

BACKGROUND OF THE INVENTION

Increasingly accurate yet fast methods and instrumentation for measuring various quantities are required in environmental analysis and technologies, in industrial monitoring, in diagnostics for health care, and in pharmacology. Some of these requirements are outlined in Parker S. (Ed.): *McGraw-Hill Encyclopedia of Chemistry*, McGraw-Hill, 1983, and in D. A. Skoog and J. J. Leary, *Principles of Instrumental Analysis,* 4th edition, Harcourt Brace College Publishers, New York, USA, 1992. For example, in environmental applications, there is a need for integrated and miniaturized measurement tools which can be used directly at sites where measurements are important (factory exits, waste, dumps etc.), and to transmit continually, without cable connection, the information necessary for real-time monitoring to the centers for pollution prevention or waste management. Amongst the most widespread methods for identification of the pollutants are those of spectrometry and in particular of absorption spectrophotometry. Numerous examples of existing needs for light-spectrum-measurement based in situ applications are described in the prior art.

Spectroscopy is an analytic technique concerned with the measurement and characterization of the interaction of radiant energy with matter. This often involves working with instruments designed for this purpose, called spectrometers, and corresponding methods of interpreting the interaction both at the fundamental level and for practical analysis. The distribution of radiant energy, absorbed or emitted by a sample of a substance under study, is called its spectrum. If energy of ultraviolet (UV), visible (Vis) or infrared (IR) light is used, the corresponding spectrum is called a light-spectrum. In the description, which follows, the term spectrum is used in the sense of light-spectrum and the term spectrometer is used in the sense of spectrophotometer.

A spectrometer has a resolution associated with its design or implementation affecting resolution of measured spectra. As is well understood by those of skill in the art of spectrometry, a required resolution for UV and a required resolution for IR spectral imaging is different. Further, the terms high-resolution and low-resolution are related to an imaged spectral band or to wavelengths of light within the imaged band. For a broadband spectrometer, either graduated spectral resolution or a spectral resolution sufficient to properly image each band is used.

Interpretation of spectra provides fundamental information at atomic and molecular energy levels. For example, the distribution of species within those levels, the nature of processes involving change from one level to another, molecular geometries, chemical bonding, and interaction of molecules in solution are all studied using spectrum information. Practically, comparisons of spectra provide a basis for the determination of qualitative chemical composition and chemical structure, and for quantitative chemical analysis as disclosed in Parker S. (Ed.): *McGraw-Hill Encyclopedia of Chemistry*, McGraw-Hill, 1983 which is hereby incorporated by reference.

Referring to information from that text, a general functional block diagram of a spectrometer is shown in FIG. **1** and contains five components:

- a stable source of radiant energy;
- a transparent container for holding the sample of the substance for analysis;
- a device that isolates a restricted region of the spectrum for measurement;
- a radiation detector which converts radiant energy to a usable signal in the form of an electrical signal; and,
- a signal processor and readout, which displays the electrical signal on a meter scale, a cathoderay tube, a digital meter, or a recorder chart.

The modem spectrometers are very sophisticated and guarantee excellent measurement performance in a laboratory environment, but in situ applications of spectrometers are only made in exceptional circumstances, since they require relatively expensive equipment, which is usually transported in special vehicles.

In general, the precision of spectrometers is considered adequate for most laboratory applications and, therefore, recent efforts in improving spectrometers have focused on improving in situ usability.

The miniaturization of spectrometers is a necessary precondition for their mass in situ application; however, the size of a spectrometer is limited by required precision and accuracy of measurements because of existing relations between optical spectral resolution, spectral range of a spectrometer and its physical dimensions. The optical spectral resolution of commonly manufactured spectrometers is proportional to their dimensions. This is a noted and important limitation for miniaturization of spectrometers, which heretofore could not be circumvented. Unfortunately, since precise spectrometers for use in environmental analysis are often bulky, costly, and expensive to transport and install, many known and important applications of spectrometers remain unimplemented due to cost and/or inconvenience. A portable spectrometer that has a lower cost than conventional spectrometers and is preferably hand-held would allow the use of spectrometers in a wide range of applications to the benefit of many industries.

Existing spectrometers, which could be adapted to in situ measurements, are relatively large and expensive. Companies such as Ocean Optics, CVI Laser Corporation, and Control Data offer miniaturized PC-compatible, on-card spectrometers whose price ranges between $6,000 and $20,000. These spectrometers are commonly intended for laboratory applications and offer interesting metrological characteristics. Some other companies offer portable autonomous spectrometers for measuring specific substance contents (e.g. Clean Earth). Their dimensions are relatively large and prices reach several thousands US Dollars. Attempts to implement the optical functions using semniconductor-based integration technologies have resulted in lower quality of operation over that-obtained by means of classic discrete technologies. Therefore, an autonomous, integrated spectrum-measurement-based tools for UV-Vis-IR range are still not available.

Recently, increased research activity is directed towards developing spectrometers for sensing applications and for wavelength division multiplexing (WDM) in optical communication; however, a simple low cost solution with a totally integrated opto-electronic part using standard technologies is still lacking. A variety of spectrometric probes for in situ measurement are known in the art. U.S. Pat. No. 5,712,710 for example, describes a probe for use in mea-