Introduction to FT-NIR Spectroscopy

Bruker Italia Srl, Optics BU

lunedì 30 maggio 2016

Spectroscopy
Introduction

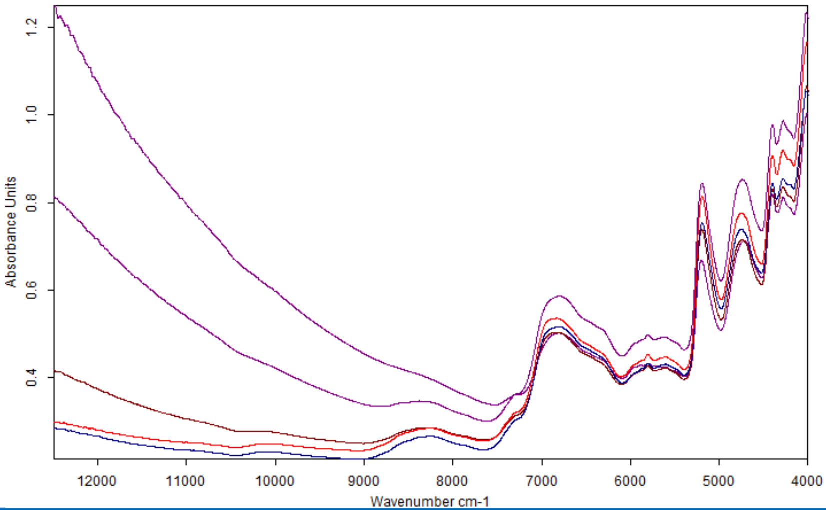
- **Spectroscopy** is a term related to the **measurement** and the **study** of a electromagnetic spectrum.
- The term **spectrum** is referred to a graphical bidimensional representation of a peaks sequence with proper **intensity** (variable along y-axis) in a certain **position** (x-axis).
- Peaks are also termed **bands**.

Spectroscopy
The spectrum

- Typically, the peak **position** (*x-axis*) is the graphical representation of a peculiar space (wavenumber, energy, wavelength).
- The peak sequence (with a precise position) represents, often, the molecules' **fingerprints**.
- The spectrum give us the possibility to read the fingerprint pattern of a sample, in order to identify it in **non** ambiguous way.
- The peaks intensity **is not** relevant for identification, but it is crucial for quantification, depending the height of a peak from the amount of sample, i.e. from the **concentration.**

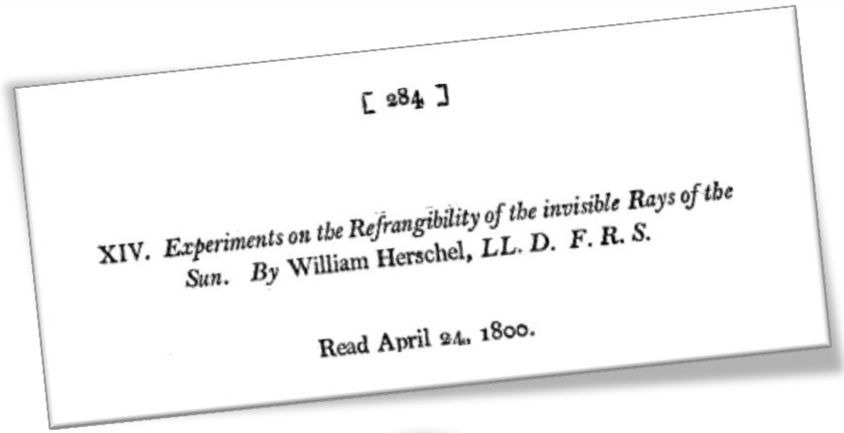
Spectroscopy and spectrometry

- From a practical approach, it is possible to get a spectrum using a **spectrometer**.
- Generally speaking, a spectrometer is a instrument able **to measure** a spectrum, by definition.
- A spectrometer able to measure the electromagnetic spectrum, i.e. the light properties in function of the wavelength, has termed **spectrophotometer**.



Spectophotometry
Dispersion

- The dispersion of light has been discovered in 1800 by astronomer Friedrich Wilhelm Herschel analyzing the spectrum of sunlight
- Large part of spectrophotometers on the market uses the inference principle to separate the electromagnetic radiation into all the composing wavelengths, measuring the intensities with a proper detector.

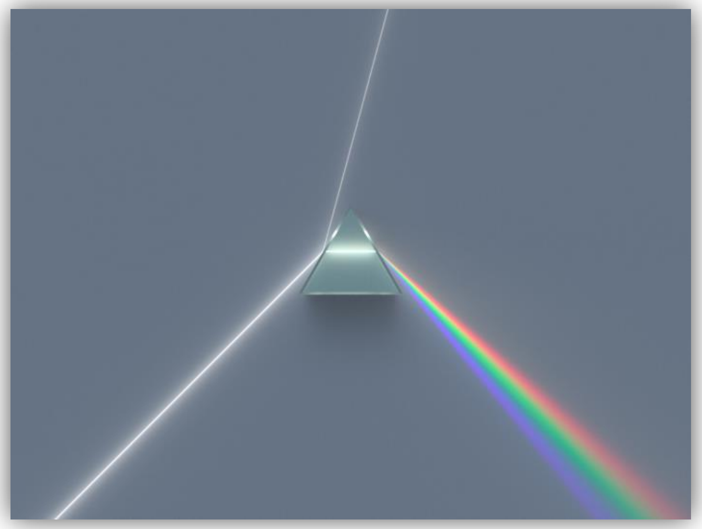

[284]

XIV. *Experiments on the Refrangibility of the invisible Rays of the Sun.* By William Herschel, LL. D. F. R. S.

Read April 24, 1800.

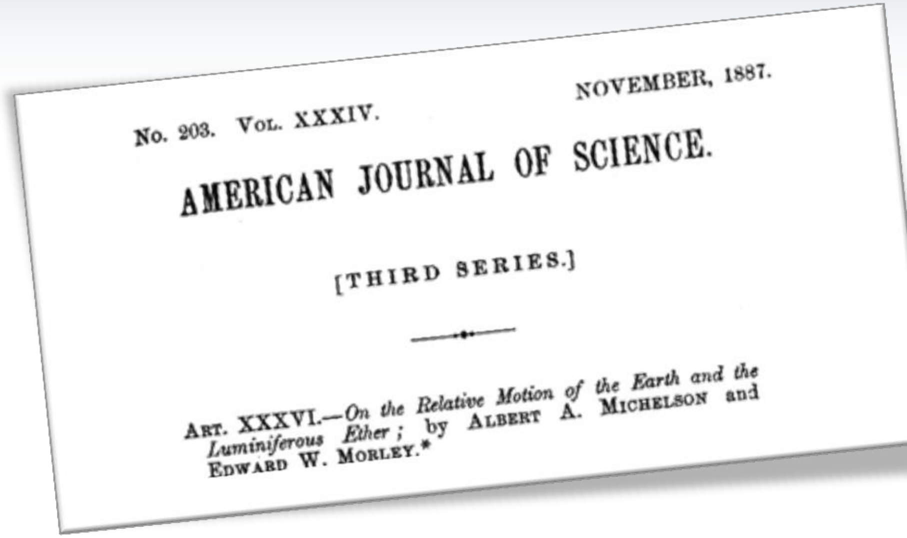
Spectrophotometry
Accuracy and Calibration

- The spectrophotometer **must ensure** that the peaks position is reproducible within a certain **accuracy** and **always** comparable with peaks tables in bibliography, in order to get an **unambiguos** results.
- A critical point is the **calibration** system used.
- Every spectrum needs to be calibrated for **every** decomposed wavelenght.



FT-IR Spectometer
The interferometer

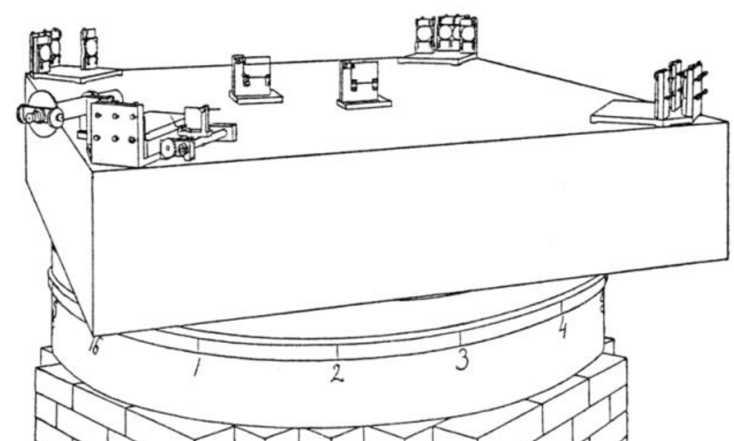
- Every FT-IR spectrometer uses an interferometer to generate the wavelength dispersion
- The interferometer is an optical device, formally invented into 1887 by Michelson and Morley


No. 203. Vol. XXXIV. NOVEMBER, 1887.

AMERICAN JOURNAL OF SCIENCE.

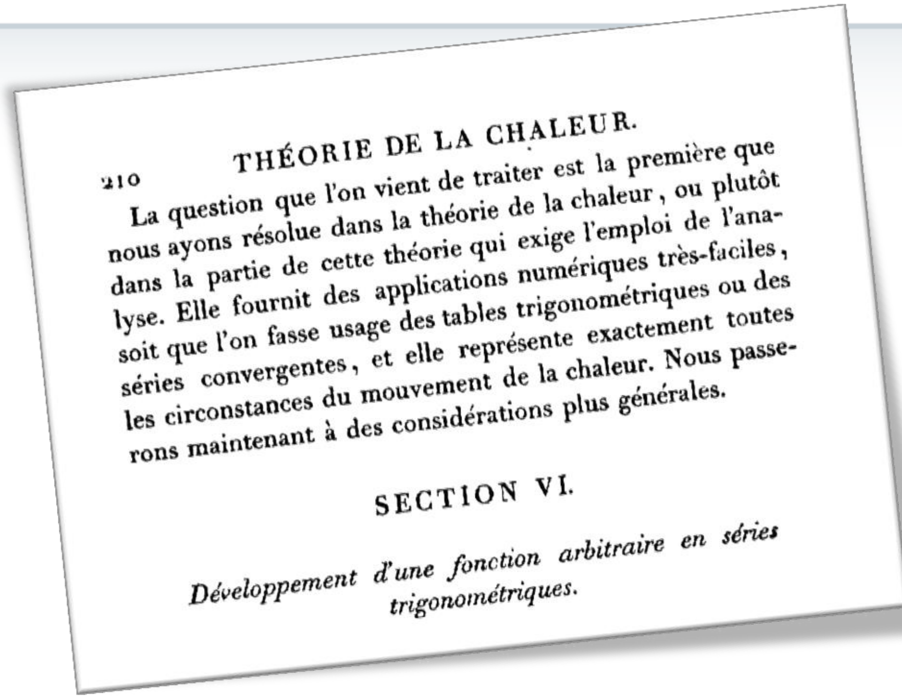
[THIRD SERIES.]

Art. XXXVI.—*On the Relative Motion of the Earth and the Luminiferous Ether*; by Albert A. Michelson and Edward W. Morley.*



FT-IR Spectometer
Fourier Transformation

- Into FT-IR spectrometry the spectrum is the final result of the **application** of Fourier Transformation to the raw data acquired from the spectrometer
- The Fourier Transformation (FT) is a mathematical operation invented into 1822 by Jean Baptiste Joseph Fourier
- If the raw data are acquired as space dependent (i.e. in function of *cm*), the spectrum will be a function of cm^{-1}, i.e. the **wavenumber**



210 THÉORIE DE LA CHALEUR.

La question que l'on vient de traiter est la première que nous ayons résolue dans la théorie de la chaleur, ou plutôt dans la partie de cette théorie qui exige l'emploi de l'analyse. Elle fournit des applications numériques très-faciles, soit que l'on fasse usage des tables trigonométriques ou des séries convergentes, et elle représente exactement toutes les circonstances du mouvement de la chaleur. Nous passerons maintenant à des considérations plus générales.

SECTION VI.

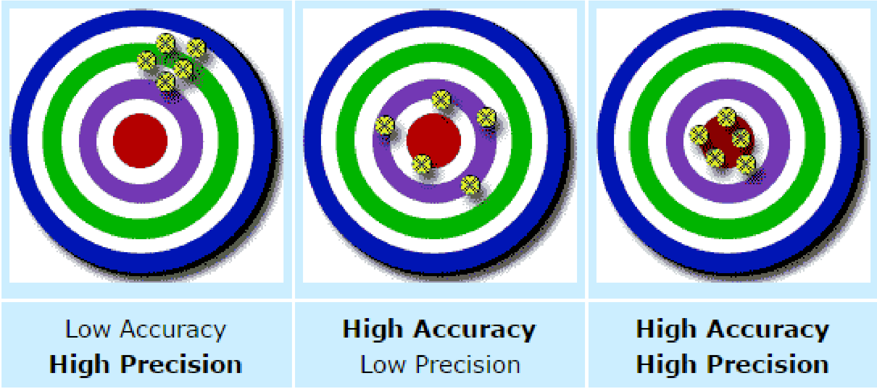
Développement d'une fonction arbitraire en séries trigonométriques.

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_0^\infty F(\omega)\, e^{i\omega t}\, dt$$

FT-IR Spectrometry
Advantages

The advantages respect to other non interferometer based tecniques are the following:

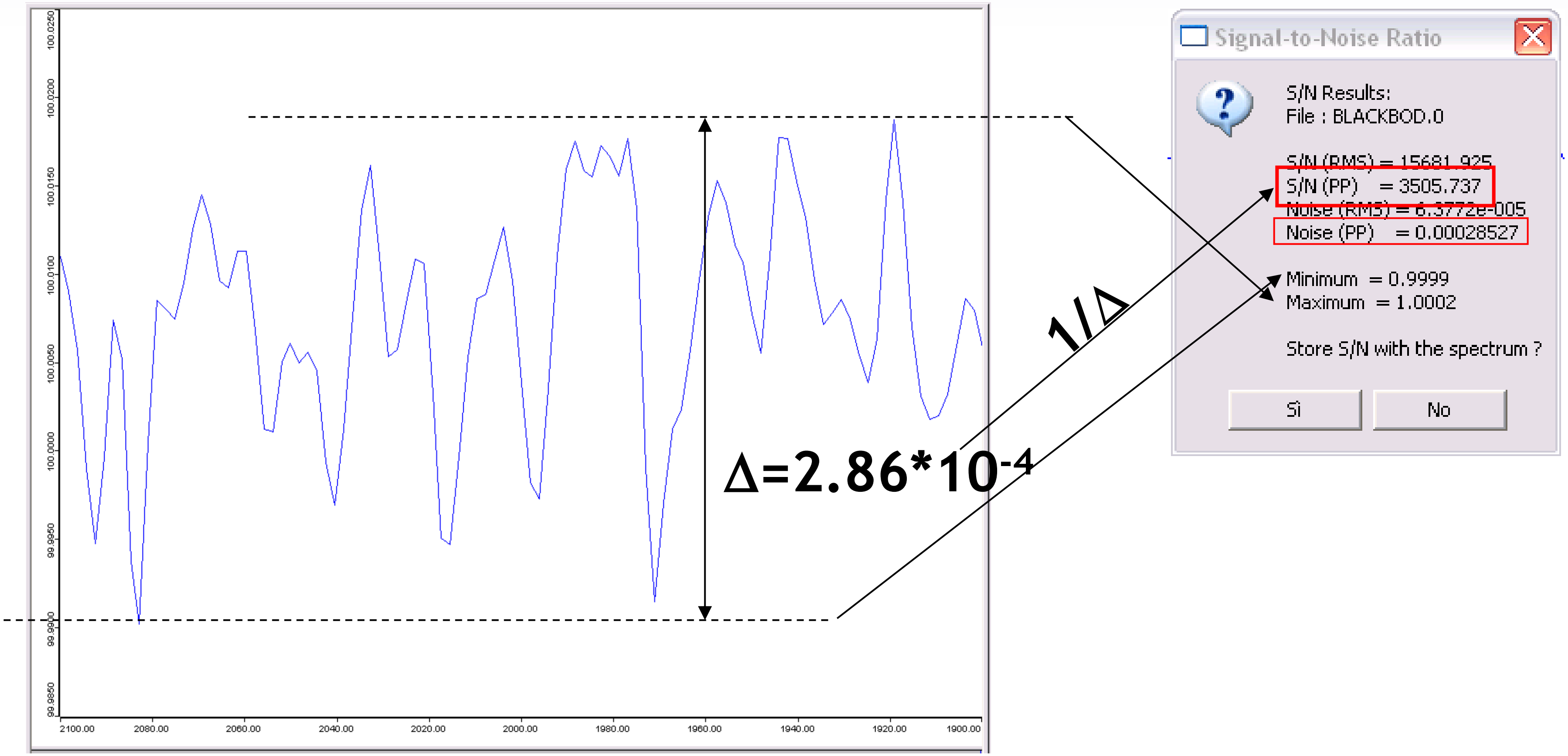
- High **accuracy** (how close a measured value is to the true value)
- High **precision** (how close the measured values are to each other)
- High Energy throughput, high **Signal to Noise Ratio** (SNR)



The high wavenumber accuracy allows a easy calibration transfer

It seems to be the ideal technique to be applied to multivariate analysis

S/N ratio



2100.00
2080.00
2060.00
2040.00
2020.00
2000.00
1980.00
1960.00
1940.00
1920.00
1900.00
Δ=2.86*10-4
1/Δ
Signal-to-Noise Ratio
S/N Results:
File : BLACKBOD.0
S/N (PP) = 3505.737
Noise (PP) = 0.00028527
Minimum = 0.9999
Maximum = 1.0002
Store S/N with the spectrum ?
Sì
No

S/N ratio:

Signal power on the DTC (Planck's law)

Acquisition time

Optical resolution

Efficiency

$$SNR = \frac{U_{\tilde{\nu}}(T) \cdot \Theta \cdot \Delta\tilde{\nu} \cdot \sqrt{t} \cdot \xi \cdot D^{*}}{\sqrt{A_D}}$$

Detectivity

DTC area

Innovation with Integrity