CLAIMS

1.- Method for determining at least one absorption band in a spectrum, the spectrum being the evolution of a absorption quantity with regard to a wavelength quantity in a predefined range of wavelength quantity, the absorption quantity being a quantity representative of the absorption and the wavelength quantity being a quantity representative of the wavelength, each absorption band being a distribution profile associated to at least one covalent bond of chemical species present in a sample, the distribution profile being characterized by mathematical parameters, the method at least comprising the steps of:

- providing a measured absorption spectrum from the sample,
- providing a calculation spectrum which is equal to the measured absorption spectrum,
- from the calculation spectrum, extracting at least one absorption band,
- forming an absorption band population by grouping each extracted absorption band,
- calculating a residual spectrum by removing each extracted absorption band from the calculation spectrum,
- testing whether a predefined stop criterion is fulfilled by the residual spectrum,
- if the stop criterion is not fulfilled, using the residual spectrum as the calculation spectrum and iterating the extracting step, the forming step, the calculating step and the testing step, the extracted absorption band(s) at the end of the iterating step being different from the previously extracted absorption band(s), and
- if the stop criterion is fulfilled, outputting each extracted absorption band.

2.- Method for determining at least one absorption band according to claim 1, wherein the distribution profile is chosen among a Gaussian profile, a Lorentzian profile and a Voigt profile, the Voigt profile being characterized by a Gaussian proportion and a Lorentzian proportion.

3.- Method for determining at least one absorption band according to claim 1, wherein the extracting step comprises the steps of:

- searching the absorption band(s) in the calculation spectrum, to obtain found absorption band(s), and
- deducing values to mathematical parameters of each found absorption band, to obtain deduced parameters.

4.- Method for determining at least one absorption band according to claim 3, wherein the extracting step comprises carrying out a step chosen in the group consisting of:

- obtaining the maxima of the calculation spectrum,
- calculating the first derivative of the absorption quantity with relation to the wavelength quantity, to obtain a first derivative of the calculation spectrum,
- calculating the second derivative of the absorption quantity with relation to the wavelength quantity, to obtain a second derivative of the calculation spectrum, and
- obtaining the minima of the second derivative of the calculation spectrum, the second derivative being the second derivative of the absorption quantity with relation to the wavelength quantity.

5.- Method for determining at least one absorption band according to claim 3, wherein, a mathematical parameter is the position of the absorption band, the position being the wavelength quantity of the absolute maximum of absorption quantity of the considered absorption band.

6.- Method for determining at least one absorption band according to claim 3, wherein, one parameter of the mathematical parameter is the width of the absorption band.

7.- Method for determining at least one absorption band according to claim 1 when depending from claim 3, wherein the extracting step further comprises:

- curve-fitting each absorption band by using the deduced parameters of the absorption band and a distribution profile.

8.- Method for determining at least one absorption band according to claim 1, wherein the stop criterion is chosen in a group consisting of:

- the integral of the absorption quantity in the residual spectrum over the predefined range of wavelength quantity is strictly inferior to the product of 1% with the integral of absorption quantity in the measured absorption spectrum over the predefined range of wavelength quantity,
- the integral of the absorption quantity in the residual spectrum over the predefined range of wavelength quantity is strictly inferior to the product of

0.1% with the integral of absorption quantity in the measured absorption spectrum over the predefined range of wavelength quantity,

- the absolute value of the absorption quantity per wavelength quantity in the residual spectrum is strictly inferior to the product of 1% with the absolute value of absorption quantity per wavelength quantity in the measured absorption spectrum,
- the absolute value of the absorption quantity per wavelength quantity in the residual spectrum is strictly inferior to the product of 0.1% with the absolute value of absorption quantity per wavelength quantity in the measured absorption spectrum,
- the ratio between the absorption quantity in the residual spectrum and the absorption quantity in the measured absorption spectrum is strictly inferior to 1% in the predefined range of wavelength quantity,
- the ratio between the absorption quantity in the residual spectrum and the absorption quantity in the measured absorption spectrum is strictly inferior to 0.1% in the predefined range of wavelength quantity, and
- any combination of the previous stop criteria.

9.- Method for determining at least one absorption band according to claim 1, wherein the method further comprises if the stop criterion is not fulfilled, a step of correcting each previously extracted absorption band by using the residual spectrum.

10.- Method for determining at least one absorption band according to claim 9, wherein each absorption band has a position and a width with extremities, the correcting step comprising, for each extracted absorption band, determining the algebraic sign of the residual spectrum at the position of the considered absorption band and/or at the extremities of the width of the considered absorption band.

11.- Method for determining at least one absorption band according to claim 9, wherein each absorption band has a position and a width with extremities, the correcting step comprising, for each extracted absorption band, analyzing the symmetry of the residual spectrum with relation to the position of each considered absorption band.

12.- Method for determining at least one absorption band according to claim 9, wherein the stop criterion is fulfilled when using the residual spectrum as the calculation spectrum to iterate the extracting step, the forming step, the calculating step and the

testing step, the previously determined bands parameters are not further modified and no new band is added to the previously obtained absorption band population.

13.- Method for three-dimensional imaging a three-dimensional sample, the method comprising at least the step of :

- dividing the three-dimensional sample in a plurality of two-dimensional samples,
- carrying out the method for determining at least one absorption band to each two-dimensional sample, the method being according to claim 1, to obtain at least one absorption band associated to at least one covalent bond for each two-dimensional sample, and
- reconstructing the three-dimensional sample by using the obtained absorption band for each two-dimensional sample.

14.- Spectrometer comprising a radiation source, optics to transport the radiation emitted by the radiation source towards the sample, a sample holder, a detector and a calculator adapted to carry out a method for determining according to claim 1.

15.- Spectrometer comprising a radiation source, optics to transport the radiation emitted by the radiation source towards the sample, a sample holder, a detector and a calculator adapted to carry out a method for three-dimensional imaging according to claim 13.

16.- Computer program product comprising a computer readable medium, having thereon a computer program comprising program instructions, the computer program being loadable into a data-processing unit and adapted to cause execution of a method for determining according to claim 1 when the computer program is run by the data-processing unit.

17.- Computer program product comprising a computer readable medium, having thereon a computer program comprising program instructions, the computer program being loadable into a data-processing unit and adapted to cause execution of a method for three-dimensional imaging according to claim 13 when the computer program is run by the data-processing unit.