



Non-Dispersive Infrared Spectrometry as a Means of Research in Geochemistry of Carbon

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Isotope geochemistry makes use of variations of stable isotopes in their natural occurrences. Such variations are either due to isotope effects, i.e. differences in physical or chemical properties of isotopes of one and the same element, or to nuclear processes initiated by cosmic radiation or by radiation emitted by natural radioactive isotopes. Finally products of decay processes of radioactive isotopes occurring in nature can also alter the isotopic composition of chemical elements in nature.

Generally the isotopic composition of chemical elements in their natural occurrences can contain and usually does contain information about the sources they stem from, and the processes taking place on the way from their origin to the present location. In case of carbon variations in isotopic composition are solely due to isotope effects.

The main processes causing isotope fractionation in nature are:

- isotope exchange reactions, particularly isotope exchange reactions between gases and liquids or solids, respectively
- kinetic isotope effects due to differences in the rate of chemical reactions
- isotope effects in diffusion
- isotope effects connected with changes of the state of aggregation (solid, liquid, gaseous)

Important processes causing fractionation of carbon isotopes in nature are:

- isotope exchange between gaseous carbon dioxide and hydrogen carbonate and carbonate, respectively, dissolved in water
- isotope exchange between gaseous hydrocarbons and hydrocarbons dissolved in natural oil
- isotope exchange between gaseous hydrocarbons and rocks
- kinetic isotope effects connected with the assimilation of atmospheric carbon dioxide by C₃-, C₄- and CAM-plants
- isotope effects which accompany migration of natural gas
- isotope effects connected with the formation of coal, natural oil and gas

Use of non-dispersive infrared spectrometry for determining stable isotopes in Geosciences: The δ -values of carbon in its natural abundances range from +4.9‰, (carbonates) to -55‰, (methane). Just organic matter extends from -15 to -55‰, methane from -25‰, to -55‰, in dependence on its metamorphic grade. In view of such wide ranges of $\delta^{13}\text{C}$ -values the moderate accuracy of non-dispersive infrared spectrometry is sufficient for many purposes of monitoring, screening and measuring carbon-containing matter in nature, particularly because small differences in isotopic composition (a few permil and smaller) are accidental rather than conform with natural laws.

With our device standard deviation of $\delta^{13}\text{C}$ -values is 0.4‰, and maximum deviation of $^{12}\text{CO}_2$ -values 0.2 vol-%.

There are three possibilities to get the sample gas from the material to be investigated:

1. Measuring air samples directly using a special spectrometer configuration
2. Pre-connecting a combustion unit, e.g. an elemental analyzer
3. Application of a trap unit for purification

With a) sampling is simple and fast, but the characteristics of non-dispersive infrared spectrometers induce some difficulties resulting from gases like oxygen and water vapor, especially if they are present in changing concentrations.

Design b) enables to examine solid and liquid substances and has the advantage to pre-separate the different components of the respective samples.

Unit c) is able to eliminate the disadvantages of configuration a) by cleaning the sample to be measured from interfering substances. Additionally, in cases a) and b) it is possible to overcome difficulties arising from low sample concentrations.

In comparison to IRMS non-dispersive infrared spectrometry is a low expenditure means of monitoring and screening $\delta^{13}\text{C}$ -values near and in the natural range with an accuracy sufficient for many purposes in geosciences and environmental research.