Gas Analysis by Mass Spectrometry

Gas analysis by mass spectrometry (MS) provides qualitative and quantitative analyses of gases and gas mixtures. It can also be used for the qualitative and quantitative analysis of volatile organic liquids.

Principle of Technique

In a gas mass spectrometer, the sample is bombarded under vacuum with an electron beam from a thoriated iridium filament. The interaction of the analyte with the electron beam forms charged species and ruptures chemical bonds, forming charged fragments of the original molecule. The type and amount of fragment ions obtained are characteristic of the molecule bombarded. Each compound will have a unique fragmentation pattern, or mass spectrum. Ions are accelerated through a constant electrostatic field and a varying magnetic field. They follow curved paths to pass through an exit slit and strike a collector. Variation of the magnetic field causes an ion of a specific mass-to-charge (m/e) ratio to impinge on the collector, thus producing a small electric current that is a measure of the amount of the specific component present in the sample. Quantitative analysis is achieved by comparison with suitable reference gas standards.

Samples

Form. Only gases or volatile liquids can be analyzed.

Size. A few grams of pressurized gas are usually sufficient, but the amount varies with the type of analysis.

Preparation. Sampling containers must be compatible with the gas analytical instrument. Guidance is available upon request.

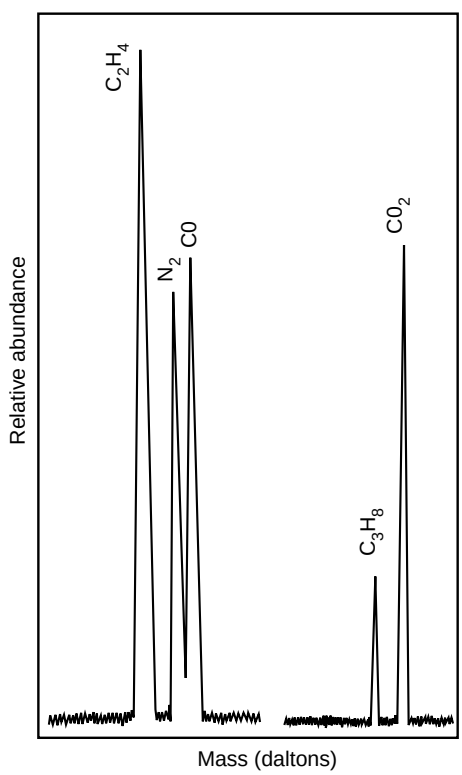
Limitations

Components of interest must be volatile. It can be difficult to identify the components of complex organic mixtures, and the analysis of halogens and water is not possible.

Certain very reactive or corrosive gases may be too unstable for sampling and quantitative introduction into the instrument. Detection limits for stable inorganic gases are in the low parts per million.

Estimated Analysis Time

Calibration and analysis requires about 30 min to 4 h, depending on sample type and complexity.



High resolution (2500) gas mass spectrometry can resolve C_2H_4, N_2, and CO (nominal mass 28 daltons), as well as C_3H_8 and CO_2 (nominal mass 44 daltons).

Examples of Applications

- Determination of isotopic ratios of inert gases.
- Measurement of oxygen and carbon dioxide in air samples from test borings of contaminated soils.
- Quantitative analysis of oil shale retort gases.
- Verification of gas mixtures that serve as calibration standards.
- Measurement of trace levels of inert gases in samples from underground nuclear tests.
- Analysis of high purity gases for contaminants.

Capabilities of Related Techniques

Gas chromatography (GC) has a greater quantitative capability for simple organic mixtures but may require a larger sample. Combination gas chromatography–mass spectrometry and gas chromatography–mass spectrometry–mass spectrometry techniques are better than gas MS for the identification of complex organic mixtures.

Infrared (IR) and Raman spectroscopy may be applicable but require a larger sample. IR fails to detect some important inorganic gases (e.g., H_2, N_2, O_2). Neither IR nor Raman detect the monatomic inert gases. A mass spectrometer is needed if isotope ratios are desired.

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