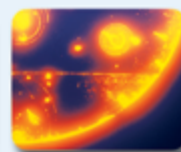
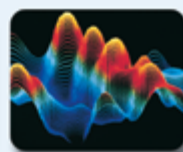


Chemistry in Action



Mass Spectrometry: Identifying Molecules

Tests for locating oil deposits in the ground and detecting dioxins in our food supply are commonly performed today. These tests can be performed by using a technique known as *mass spectrometry*. Mass spectrometry is now used in many fields, such as medicine, chemistry, forensic science, and astronomy.

What is mass spectrometry? It is the most accurate technique available to measure the mass of an individual molecule or atom. Knowing the molecular mass is an essential part of identifying an unknown compound and determining the structure of a molecule of the compound. As the diagram of a mass spectrometer shows, the molecules in a gaseous sample are converted into ions. The ions then are separated and sorted according to their mass-to-charge ratio by a combination of electric and magnetic fields. The fields cause the ions' trajectories to change based on the ions' masses and charges. Then, the sorted ions are detected, and a mass spectrum is obtained. The mass spectrum is a graph of relative intensity (related to the number of ions detected) versus mass-to-charge ratio. Mass spectrometry uses a very small sample size (10^{-12} g) to obtain results.

The resulting spectrum is like a puzzle. It contains numerous peaks that correspond to fragments of the initial molecule. The largest peak (parent peak) corresponds to the

molecular mass of the molecular ion. By analyzing the peaks, scientists can determine the identity and structure of a compound. Computers are used to help interpret the spectrum and identify the molecule by using online spectral database libraries.

Mass spectrometry has been an essential tool for scientists since its invention in the early 1900s. But its use was limited to small molecules from which ion creation was easy. Large biological molecules could not be studied because they would break down or decompose during conventional ion-formation techniques. In the late 1980s, two groups developed ion-formation methods that are used today in commercial mass spectrometers. John Fenn (Virginia Commonwealth University) developed electrospray ionization

mass spectrometry, and Koichi Tanaka (Shimadzu Corporation, Japan) developed matrix-assisted laser desorption ionization (MALDI) mass spectrometry. In 2002, both scientists received the Nobel Prize in chemistry for their work. Their methods opened the field to the study of large molecules, allowing scientists to use mass spectrometry to study the structure of macromolecules such as nucleic acids and steroids and to identify the sequence of proteins.

Questions

1. Why is it necessary to convert the sample into ions in the mass spectrometer?
2. How have recent developments in mass spectrometry contributed to the field of medicine?

▼ *Scientists use mass spectrometers to identify and study the structure of molecules.*

