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Scientific Instrumentation

Instrumentation has opened many frontiers for investigation or has sped exploration of existing fields. Improvement of analytical equipment has been especially notable. Further progress is portrayed in this issue of *Science*. Developments in mass spectrometry are particularly impressive. Mass spectroscopists have volatilized hitherto involatile substances, including some with molecular weights as high as 12,500. They can determine masses of large molecules and of their fragments and thus obtain much information about molecular weights and structure. This capability can be coupled with various forms of chromatography and gel electrophoresis. Together, these tools will be used to facilitate discoveries in many areas of biology and medicine.

In mass spectrometry beams of ions are bent, usually in magnetic fields. For a given charge, the lighter ions are deflected more readily than the heavier ones. Thus, the constituents of the beam arrive at different places on a target. Ion beams may be formed by volatilizing the substance being analyzed, bombarding the vapor with electrons to make ions, and accelerating the ions. By 1940 mass spectrometry was being used in physics (for isotopes), earth science (radiometric dating), analytical chemistry, and biochemistry.

With time, all the components of mass spectrometers have been improved, including magnet design and control and detecting equipment. Computers have been added. More efficient types of ion sources have been created. In some forms of mass spectrometry molecular weights can be determined with a precision of 5 parts per million. Substances present in the 10^{-15} mole range have been detected. The combination of gas chromatography with mass spectrometry proved very effective in identifying and quantitating components of complex mixtures such as petroleum.

Until recently, though, many important types of molecules could not be studied by mass spectrometry. These were involatile substances or materials that would be destroyed by heating them to the temperature necessary to volatilize them. Examples are carbohydrates and polypeptides.

In attempts to volatilize these substances, techniques such as field desorption and laser desorption have been used. Major success has come from bombardment of the sample by energetic charged or uncharged atoms. Results of studies with fast atom bombardment are described by Rinehart in this issue. Argon or xenon is ionized and accelerated to 3 to 10 kilovolts. The ions are neutralized and the beam is directed to target substances in a nonvolatile solvent, such as glycerol. The large molecules, often accompanied by glycerol molecules, are given sufficient energy to escape from the surface. Some of the large molecules are intact and ionized, and their masses can be measured. Some of them break into fragments, which can also be detected and measured. The fragmentation appears to occur in reproducible ways. Breaks usually occur where a heteroatom is attached to a carbon chain. Rinehart reports that when a compound containing a sugar was subjected to fast atom bombardment, peaks of molecules with and without the sugar were found. The mass difference between the peaks was 163, which corresponds to $C_6H_{11}O_5$. When polypeptides are studied, the molecular ions provide the molecular weight. Ions at low masses are characteristic of individual amino acids. Ions at intermediate masses provide information about the sequence of the amino acids. Fragmentation was observed to occur often at the CO–N bonds with charge retention on the amino terminal fragment. When a high-resolution spectrometer is employed the atomic proportions of a fragment can be determined since the mass defects of hydrogen, carbon, nitrogen, and oxygen differ.

Mass spectroscopists are already talking of further possible advances that will make their instruments even more useful in tackling scientific questions. But were their ability to be limited to exploiting the recently revealed potentialities, their contributions would still be enormous.

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