Identification of Elements and Compounds

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One of the most common activities of chemists is to determine the elements and compounds present in a sample of material. If a chemist wishes to analyze a sample to find what elements or compounds are present, that is, to identify the elements and compounds present, she or he will choose a **qualitative analysis** method. Once the species that are present in a sample is known, the analytical chemist may choose to determine how much of each species is present using a quantitative analytical method. Some methods perform both qualitative and quantitative results, but most are used for one purpose or the other.

The identification of elements and compounds is critical to all areas to which **chemistry** is applied, from **astrochemistry** and **biochemistry** to **geochemistry** and **industrial chemistry**. Hundreds of techniques for determining the identity of elements and compounds are available to chemists. The choice of a technique depends on many factors, including the physical state of the sample; the size of the sample; the level of accuracy required; and the time, money, and expertise of the staff that are available. An important objective of analytical chemists is to develop reliable, inexpensive, and rapid tests for the presence of specific compounds.

If little is known about a sample and a complete qualitative analysis is required, a great deal of effort and several sophisticated techniques may be required. More commonly, however, the question is whether a particular element or compound is present. Most of the techniques to be described below are aimed at identifying a particular element or compound or a few closely related elements or compounds.

Qualitative elemental analysis methods comprise both instrumental and chemical (or wet) techniques. Most instrumental techniques for elemental analysis are destructive. A solid or liquid sample is subjected to harsh conditions such as a high **temperature** flame or a very high voltage electric arc or spark that converts the sample to gaseous atoms, ions, or a **plasma**. Under such conditions, the resulting species may emit light, the basis for the technique of atomic emission **spectroscopy**, which is very useful for identifying the presence of a wide variety of elements. Modern atomic emission spectroscopy is a sophisticated extension of the flame tests that have been used for centuries to detect the presence of **metals** such as **sodium** and **potassium**. Elements of atomic **mass** greater than sodium can be made to emit x rays. By determining the wavelengths of the emitted x rays, many elements can be identified in a single sample simultaneously.

So-called wet techniques have been developed for many elements. They are often rapid and require little material. However, they may provide a reliable result only if the element is present in the sample in a particular form. For example, lead can be identified in a sample by the formation of a yellow precipitate when a **solution** of **sodium chloride** is added. But for this to happen, the lead must be present in the sample as soluble Pb (II) ions. If the lead is present as insoluble PbO_2, it would go undetected. If the analyst knows enough about the nature of the sample and that it is likely to contain PbO_2, she might first add sufficiently strong acid and an appropriate reducing agent to convert it to soluble Pb (II). Typically, the choice of a wet method requires specific knowledge about the sample as well as the level of accuracy required.

Identification of compounds takes two forms: determining the nature of a compound whose identity is unknown and identifying the presence of a known compound in a sample. To accurately determine the nature of an unknown compound, it must first be carefully purified by techniques such as chromatographic separation, **distillation**, or crystallization. The strategy typically begins with qualitative and then **quantitative analysis** to determine the compound's formula. Analysis of an organic compound typically begins with spectroscopic techniques such as **infrared spectroscopy** (which reveals the presence of many types of functional groups), mass spectroscopy (which can provide the molecular mass as well as indicate the presence of certain functional groups from the molecule's fragmentation pattern), and **nuclear magnetic resonance** (which can be used to deduce presence and the connectivity of functional groups). Elemental analysis is often used to confirm the **molecular formula** deduced from spectroscopic experiments.

Once the structure of an organic species has been identified, the presence of the **molecule** in other samples can be detected by using spectroscopic patterns or chromatographic characteristics of the compound. Infrared spectra and mass spectrographs of organic compounds are typically very detailed, offering a unique fingerprint that can be used to identify the presence of the compound. Chromatographic methods are very useful for determining the presence of several, usually related, organic compounds in the same sample. In the most common chromatographic analysis techniques, gas **chromatography** and high performance liquid chromatography (HPLC), a sample is injected at one end of a column with a specific coating or containing a finely divided support material, respectively, and any organic compound is detected at the exit point of the column.

A particular compound is identified in the sample if the detector indicates a compound at the same time it takes for the known compound to exit from the same column under the same conditions (for example, the same flow rate for the gas used in gas chromatography or solvent(s) used in liquid chromatography. Gas chromatography-mass spectroscopy (GC mass spec) is a widely used identification technique that combines a gas chromatograph, which separates and purifies compounds in a sample, with mass spectroscopy, which provides a fingerprint to allow rapid identification of each species. This combination is very powerful because the mass spectrogram of a complex mixture would consist of many overlapping fingerprints that could be very hard to decipher.

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