M.Sc Inorganic Chemistry
(Special-III) Elective Paper-1
Semester-IV

Course Title: Spectral Techniques in Inorganic Chemistry

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Data analysis

The usual strategy for identifying a known compound (i.e. one that has been made and characterized before) by mass spectrometry is to compare the spectrum recorded against databases that contain hundreds of thousands of fragmentation patterns of known compounds.

If, however, the compound is novel, then we must attempt to identify it manually by obtaining an accurate mass value for the molecular ion peak, which will allow

us to suggest a possible empirical formula, and then to look for clues in the fragmentation pattern that will suggest how the atoms are grouped together.

Molecular ions

A mass spectrum is plotted in the form of ion current at the detector as a function of *m/z*. The form of the spectrum depends strongly on the ion source used. EI generates many fragments, most of which carry a single positive charge, but it is quite normal to observe small numbers of doubly, or even triply, charged ions, particularly for metal complexes.

ESI generates far fewer fragments, and they are likely to be multiply charged. The simplest process occurring in a mass spectrometer involves the interaction of an electron with a molecule, resulting in the loss of a further electron from the molecule, leaving a radical cation. This ion is called the molecular ion, $M^{\cdot+}$. It has effectively the same mass as the parent molecule, less the mass of the electron, which for high accuracy work must be accounted for.

Usually it is the ion with the highest mass in the spectrum, although species with higher masses can occasionally be formed by subsequent ion-molecule reactions.

Thus it is often possible to determine the molecular weight (relative molecular mass) of a compound simply by looking for the highest mass peak in its mass spectrum.

For example, manganese carbonyl gives a parent ion at 390 Da, and as the masses of a manganese atom and a carbonyl group are 55 and 28 Da respectively, it does not take long to deduce that the actual compound must be $[Mn_2(CO)_{10}]$.