ThO-3

MSMS OF CARBON-13 ISOTOPES AN AID FOR ELEMENTAL COMPOSITIONS

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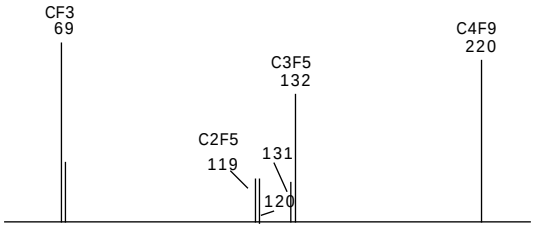

Recognise this mass spectrum? - not easy! - yet it is a spectrum of probably the most common reference compound in organic mass spectrometry - FC43 or heptacosatrifluoro-n-butylamine. This is the spectrum of the daughter ions of the peak at 220 daltons.

Yes - 220 is not well known - it is the carbon-13 isotope peak of the well known 219 peak(C4F9). Interesting is that the daughter ions consist of pairs of masses. This is because the daughters may or may not include the carbon-13 atom from the 220 ion. Also interesting is the relative intensities of each pair.

69/70 = 3:1; 119/120 = 1:1; 131/132 = 1:3.

Why is this? Little exercise for you.

These results hint that it may be possible to predict the number of carbon atoms in any parent ion just from the relative intensities of the pairs of daughter ions provided one has a rough idea of this number to start with. Also there is a redundancy of information here which can be useful when practical measurements of relative intensity which contain some error are used.

We have used 2 mass spectrometers (Finnigan/Thermo GCQ and Finnigan/Thermo TSQ700) to test the usefulness of this idea in predicting the numbers of carbon atoms in various molecules

Both mass spectrometers get good answers from probe samples. The TSQ700 has better accuracy in measuring the relative heights of the pairs of peaks but can have problems if high collisional energies are used. A Basic computer program can be used to accommodate multiple intensity ratios with less accurate results. This has proved useful for predicting numbers of carbons and hence elemental compositions for compounds from GC peaks on both the GCQ and TSQ700 mass spectrometers.