Interpretation of Mass Spectra (Fourth Edition)

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Standard Interpretation Procedure

1. Study all available information (spectroscopic, chemical, sample history). Give explicit directions for obtaining spectrum. Verify m/z assignments.
2. Using isotopic abundances, where possible deduce the elemental composition of each peak in the spectrum; calculate rings plus double bonds.
3. Test molecular ion identity; must be highest mass peak in spectrum, odd-electron ion, and give logical neutral losses. Check with CI or other soft ionization.
4. Mark “important” ions: odd-electron and those of highest abundance, highest mass, and/or highest mass in a group of peaks.
5. Study general appearance of spectrum; molecular stability, labile bonds.
6. Postulate and rank possible structural assignments for:
   (a) important low-mass ion series;
   (b) important primary neutral fragments from M⁺ indicated by high-mass ions (loss of largest alkyl favored) plus those from secondary fragmentations indicated by CAD spectra;
   (c) important characteristic ions.
7. Postulate molecular structures; test against reference spectrum, against spectra of similar compounds, or against spectra predicted from mechanisms of ion decompositions.