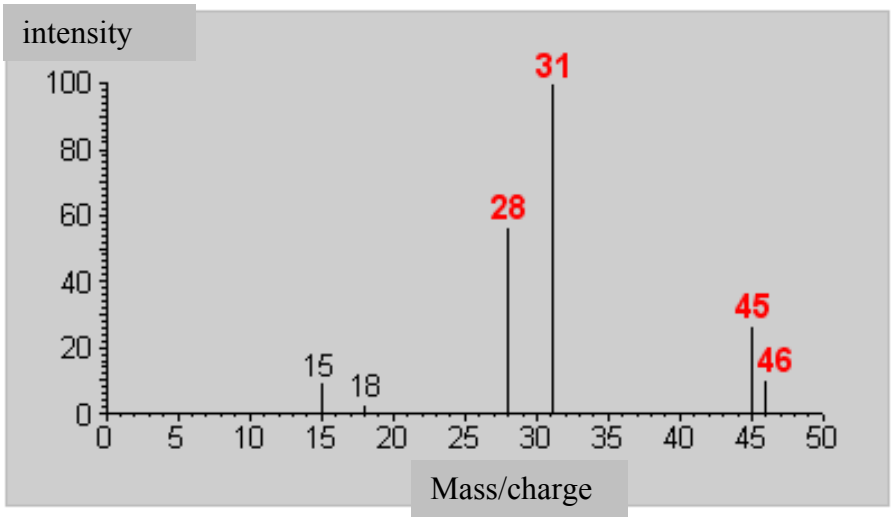
Exercises EI-MS:

1. Something easy at the beginning:

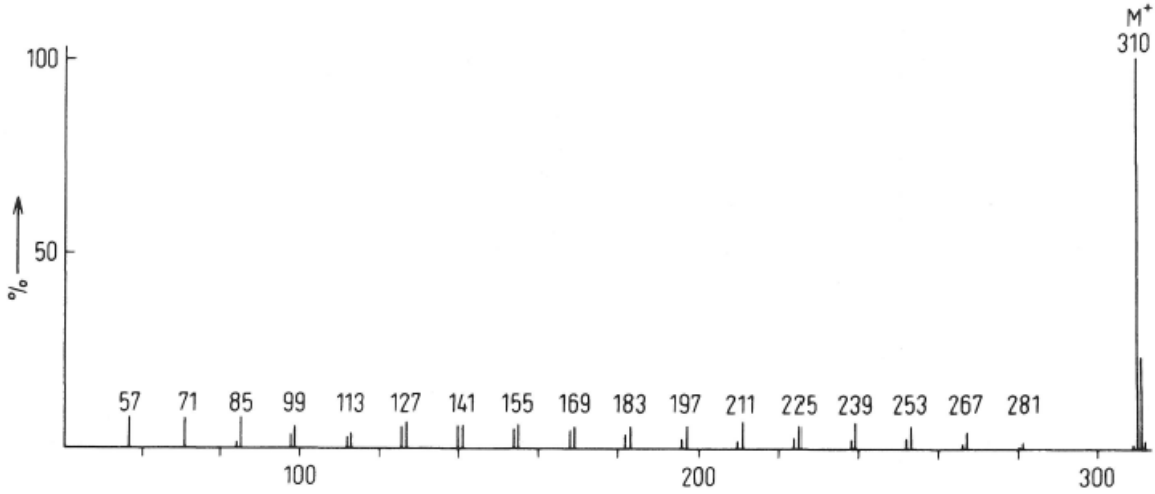


a) What is the substance (elemental composition and structure)? What can be said using the nitrogen rule?

b) Please assign structures to the different signals and think about the way of formation!

c) Why this mass spectrum is not that easy to solve?

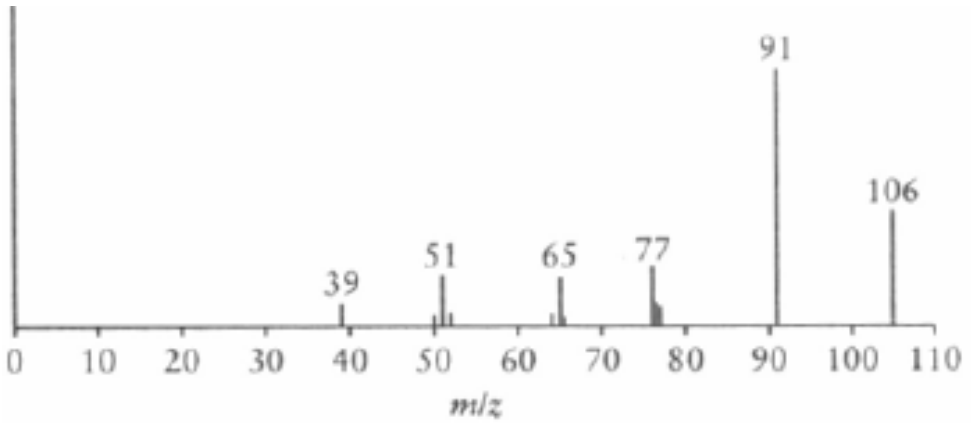
2. A bit more difficult:



EI, but with comparably low ionization energy (17.5 eV). At standard ionization energy, the $M^{+\bullet}$ would not be seen.

Questions: What kind of molecule is it? What is the structure (according to the fragmentation pattern)?

3. and now … one more example



Questions:

a) What is the elemental composition of the substance (m/z 106 = $M^{\bullet+}$)? How many double bond equivalents are in the molecule?

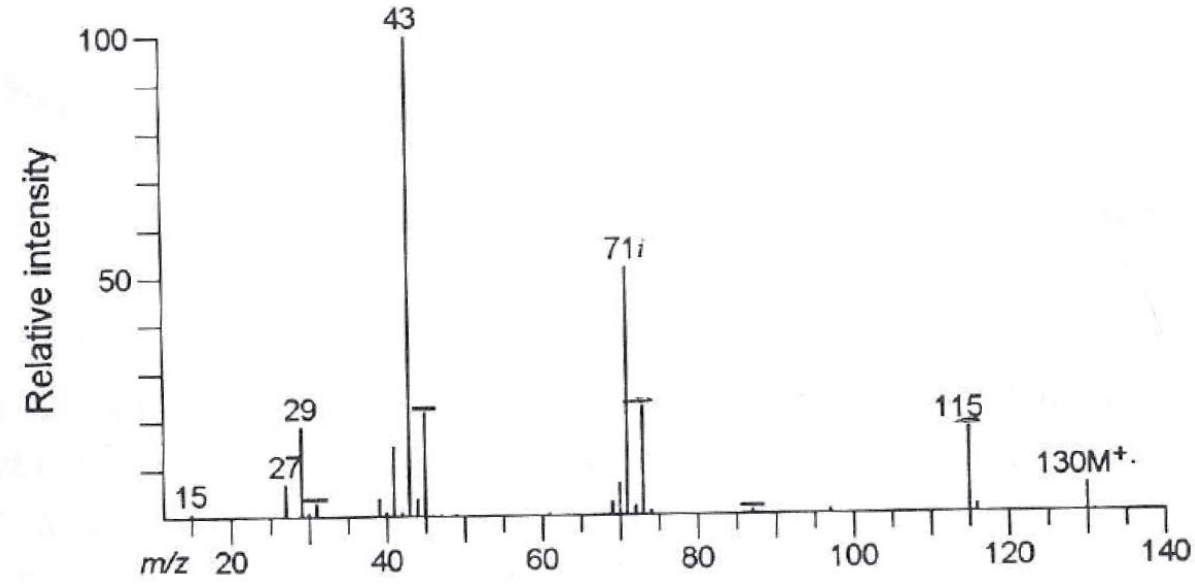
b) What are the elemental compositions of the fragment ions? What structures would you suggest?

m/z 39 m/z 51 m/z 65

m/z 77 m/z 91

c) How m/z 77 is formed?

4. One more:

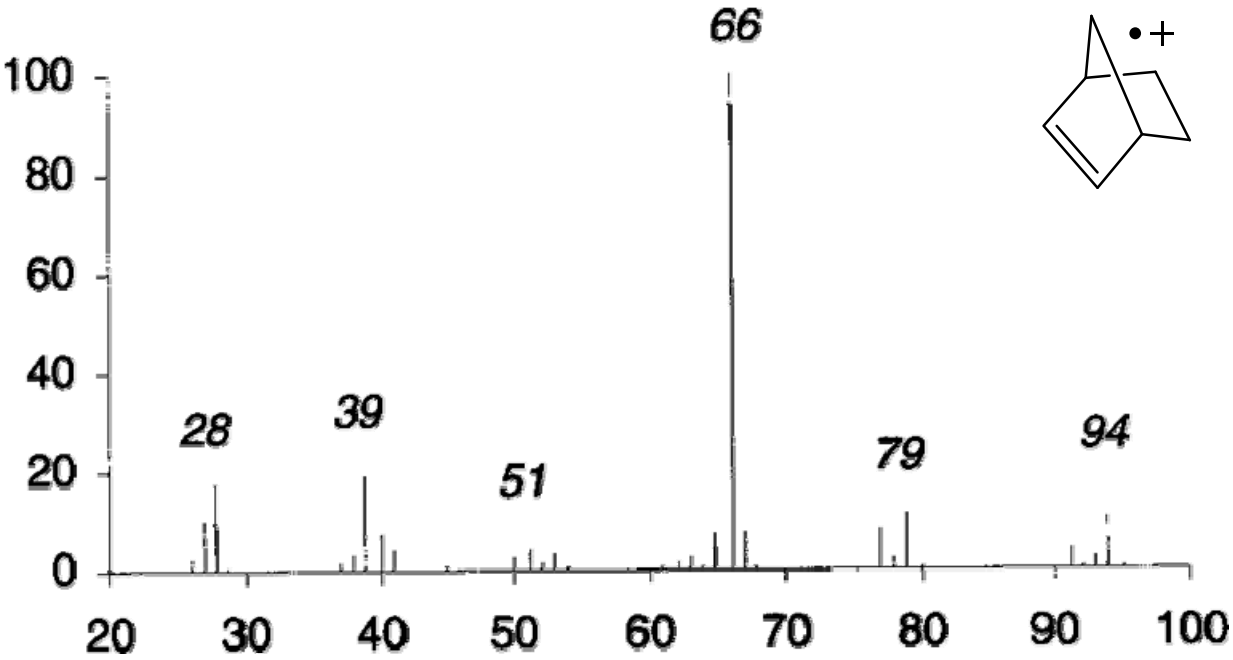


Task: assign the structure of the ether according to the mass spectrum above.

Additional to the peaks picked in the spectrum, m/z 31, 45, and 73 can be assigned.

Please also mark out the mechanisms.

5. Looks more difficult than it is:



a) How do the fragment ions look like? Please assign elemental compositions, structures if possible!

b) How the ion with m/z 66 is formed? (mechanism)

Literature:

F. W. McLafferty, F. Tureček: *Interpretation of Mass Spectra*, University Science Books; 4th edition (May, 1993) ISBN 0-935702-25-3

J. H. Gross: *Mass Spectrometry: A Textbook*, Springer Verlag, 2st edition (June, 2006) ISBN-10: 3-540407-39-1

http://www.colby.edu/chemistry/NMR/NMR.html (Tools for calculation of elemental compositions derived from (fragment-) masses, isotopic distributions, and so on. Also tools for NMR, IR) http://www.chem.uni-potsdam.de/tools/index.html (same)

http://webbook.nist.gov/ (data base: IR, NMR, mass spectra, physical. data, …)