# A Computer Program for Calculating Isotope Mass Spectra

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For the interpretation of mass spectra of varying complexity it will often be useful to calculate the complete mass spectra of one or several ions with contributions from all isotopic species present. For this purpose, a computer program, MSPEK,[1] has been written for UNIVAC 1108 with the EXEC-8 executive system. Source languages are NU ALGOL and FORTRAN V. Storage requirements are about 23 300 words in the program bank and 9300 words in the data bank.

Computations of ionic masses and relative intensities of the lines of a mass spectrum are performed for one or more ions of specified chemical composition. Tables of natural abundances of all stable isotopes are contained in the source program, making an updating of isotopic masses and abundances easy to perform, although no mechanism for introducing such information as input data has been included. The program output consists of a list of ionic masses and line intensities and/or a graphic presentation of the spectrum.

*Method of calculation.* All possible sets of isotopes for a given element are generated according to the number of atoms $N$ of that element in the molecule and the number of stable isotopes $M$ for the element. For a given set $\sigma$, the mass $m_\sigma$ and abundance $P_\sigma$ is given by

$$m_\sigma = \sum_{i=1}^{M} m_i N_{i\sigma}$$

$$P_\sigma = \frac{N! \prod_{i=1}^{M} P_i^{N_{i\sigma}}}{\prod_{i=1}^{M} (N_{i\sigma}!)} \qquad (1)$$

where $N_{i\sigma}$ is the number of atoms of isotope i in the set $\sigma$.

$$N_\sigma = \sum_{i=1}^{M} N_{i\sigma};\ \sigma = 1,2,\ldots, \text{number of sets.} \qquad (2)$$

When a molecule consists of $L$ different elements, isotope lines for each element can be calculated and combined. Mass and abundance for a given line are determined by

$$m = \sum_{l=1}^{L} m_{\sigma_l}$$

$$P = \sum_{l=1}^{L} P_{\sigma_l} \qquad (3)$$

where indices $\sigma_l$ denote lines in the isotope clusters for each element.

The mass spectrum calculated in this way will contain all possible lines. If the mass resolution of the spectrograph is $R$, we will assume that two peaks with masses $m_1$ and $m_2$ and abundances $P_1$ and $P_2$ will not be resolved if the unequality

$$|m_1 - m_2| < \frac{m_1 + m_2}{2R} \qquad (4)$$

is satisfied. This can be taken into account using

$$m = m_1 + |m_1 - m_2| \frac{P_2}{P}$$

$$P = P_1 + P_2 \qquad (5)$$

if the relation (4) is satisfied. In addition very small peaks will not be observed in the experimental mass spectrum, so lines of relative intensity less than .0001 are exluded. (The strongest line in the spectrum is normalized to 1.0.)

*Data I/0.* Table of ionic masses, natural abundances, and number of isotopes for the elements [2] are included in the program. All additional data are read from cards. In particular, a file of data cards, each containing a chemical formula and a weight factor, gives information about each wanted ion. For each card the chemical formula is decoded and ordered into a net formula by a subroutine TYDE, and the isotope cluster is calculated and scaled according to the weight factor. In the end all clusters are collected into a total spectrum. It is believed that TYDE will be useful for other purposes where decoding of a chemical formula is needed. The versatility of this formula interpreting routine, accepting formulas containing up to nine parenthesis levels, may be illustrated by the following example: The strings

C6CL6 (C1CL)6 ((C)(CL))6 (CL1)6(C2)3 C1CL6C5

will all be decoded as $C_6Cl_6$.

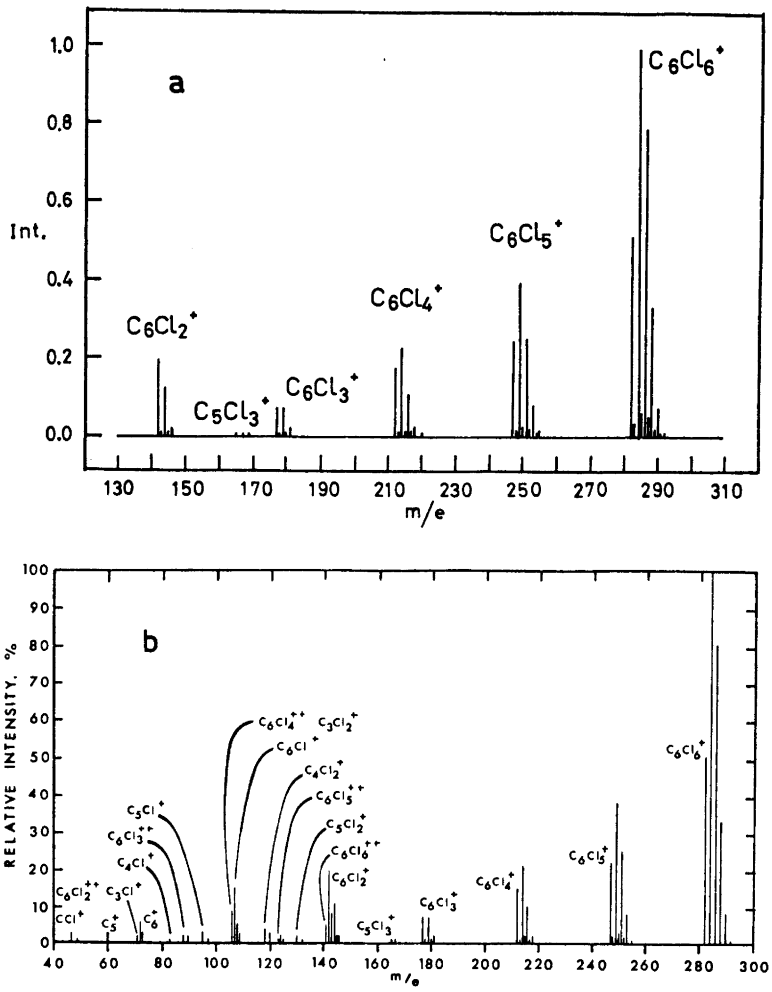


*Fig. 1.* Plot of some selected isotope clusters (a) compared with the observed mass spectrum of octachloro-3-methylenecyclopentene (b) (McLafferty, F. W. *Anal. Chem.* **28** (1956) 306).

In addition to a list of ionic masses and line intensities, a paper tape for the KINGMATIC X-Y plotter may be produced, with an optionally linear or logarithmic intensity scale.

Fig. 1 shows as an example selected isotope clusters of a calculated mass spectrum compared with an experimental spectrum of octachloro-3-methylenecyclopentene.[3]

The program may be obtained from the authors.

1. Borgen, O. and Larsen, B. *Techn. Rep. 63*, Institute of Physical Chemistry, Univ. of Trondheim-NTH 1972.
2. Condon, E. U. *Handbook of Physics*, 2nd. Ed., McGraw, New York 1967.
3. McLafferty, F. W. *Anal. Chem.* **28** (1956) 306.

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