NASA TECH BRIEF

Mass Spectograph Analysis

The problem:

The quantitative analysis of mass spectral data is a tedious and time consuming chore. When the mixture represented by the spectrum is complex or the constituents are not known, the analysis may become overwhelming if hand reductions are attempted.

The solution:

The methods used in such analyses are ideally suited to mechanization on a digital computer since they consist of the systematic search 'of a large amount of tabular data and the unknown spectra. This program provides a means of rapid data reduction of mass spectrograph data.

How it's done:

An elimination process is used to compare the unknown sample spectra with the spectra of 1519 organic compounds. Likely candidates are retained and a detailed analysis is constructed by subtraction and renormalization process. The resulting combinations of spectra are output for the user's inspection.

The method of successive subtractions, where neither the number of components nor their identities are known, is applied after two preliminary reductions are carried out. In the first reduction, the tabulated mass spectrograph data for a large number of gases are scanned, and all gases having peaks at mass numbers higher than the heaviest observed fraction in the unknown spectrum are eliminated. A second reduction in the number of possible constituents is made by rejecting all gases having a principal peak at mass numbers which, in the unknown spectrum, are less than one unit high. After execution of the two pre-liminary reductions the analysis follows a schematic technique to compare gases in reducing the spectrum by successive subtractions. Qualitative results are yielded, but for a given set of mass spectrograph data there is not necessarily a unique set of gases. The problem becomes one of searching for likely combinations of gases.

Samples are tested against other gases in the library and paths of analysis are created. The program is provided with a generous amount of output in order to facilitate the tracing of each path of analysis. The gases in the library are organized according to a serial list, all redundancies are eliminated, and the serial numbers are retained for the library.

Notes:

1. This program is written in FORTRAN IV language for use on the UNIVAC 1107/1108 system.
2. The program makes use of NASA serial numbers in its output. A list is provided in the documentation.
3. Inquiries concerning this innovation may be directed to:

> COSMIC
> Computer Center
> University of Georgia
> Athens, Georgia 30601
> Reference: B69-10134

Patent status:

No patent action is contemplated by NASA.

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