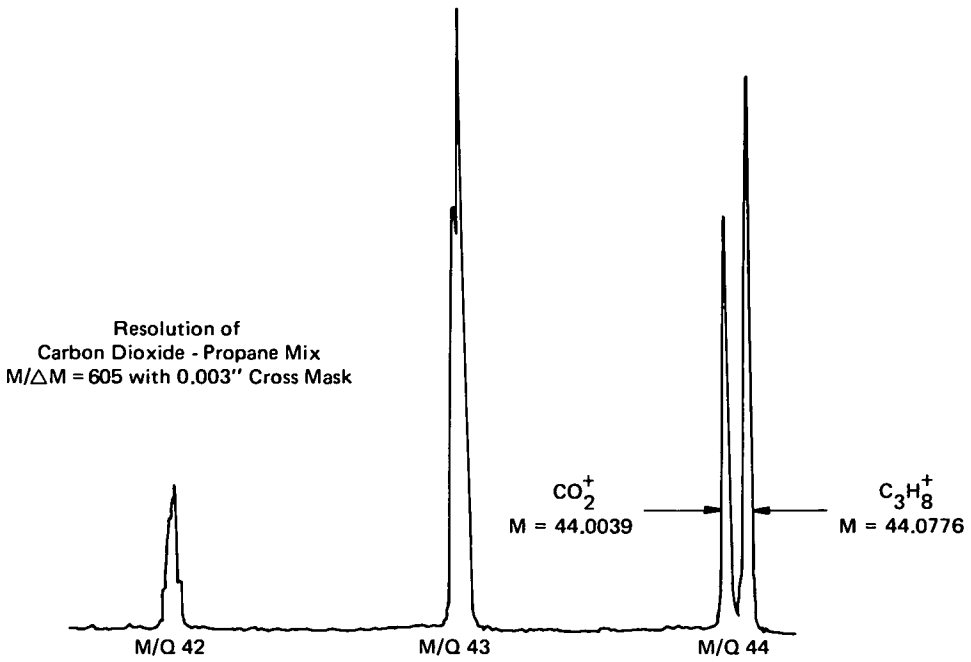
NASA TECH BRIEF

Goddard Space Flight Center

Ion Masking Improves Resolution in Quadrupole Mass Spectrometers



Resolution in Quadrupole Mass Spectrometer

A thorough experimental and computer-aided theoretical study has been made on the effects of ion masking in ion quadrupole mass spectrometry.

Mass spectrometers are used to analyze molecular composition by determining the mass-to-charge ratio (m/q) of ion fragments of the molecules. The spectrometer consists of three main parts: an ionization source to form ions from the sample, a separator to pick out ions with a specific mass/charge ratio, and an ion collector. In an ion quadrupole spectrometer, an electric quadrupole field is used to separate the desired ions.

The quadrupole field is formed by four parallel cylindrical rods on which an RF and dc potential are superimposed. The ions passing through the field oscillate. The RF/dc ratio is adjusted so that those ions of a given m/q ratio perform stable oscillations of a constant amplitude, while the remainder oscillate at increasing amplitudes and collide with the rods rather than reach the collector. However, several unstable ions do make it through the quadrupole filter and cause the m/q peaks to have significant "tails" that interfere with the resolution of the spectrometer. Parameters such as the frequency of the RF-field variation, the length of the quadrupole field, and the axial velocity of the ion can be adjusted to control the tails. But there are severe inherent limitations on the extent to which these parameters may be varied. To further improve the resolution, it is necessary to remove the unstable ions before they enter the quadrupole field.

In this study, new methods are developed for reducing peak tails. A mathematical analysis of the unstable ions shows that ions entering the quadrupole

(continued overleaf)

field near the X and Y axes (where the Z axis is in the direction of ion travel) will not be deflected by the rods. Computer simulation of the unstable ion behavior indicated that placing a cross-shaped mask over the entrance to the quadrupole field would reduce the magnitude of the tails. Based on these results, 0.005 and 0.003 inch cross masks were used with an actual spectrometer. The results were extremely good.

Resolving powers over 750 were obtained, though they required a modification of the nozzle to maintain sensitivity. In the past, resolutions of only 200 were not uncommon with this system. For instance, the accompanying illustration shows how the peaks for CO_2^+ and $C_3H_8^+$ can be resolved with this technique, a result that is not possible with this instrument without ion masking. It is also indicated that the use of angle masking may improve even these results.

The study itself adds significantly to the quantitative understanding of the quadrupole mass filter. It includes development of a quantitative theory of ion oscillations, a computer analysis of ion behavior, and the identification of the determining factors in peak tail size.

Notes:

1. The following documentation may be obtained from:
   National Technical Information Service
   Springfield, Virginia 22151
   Single document price $3.00
   (or microfiche $0.95)

   Reference: NASA CR-11578 (N71-13676), Quadrupole Ion Entrance Mask Study
2. Technical questions may be directed to:
   Technology Utilization Officer
   Goddard Space Center
   Code 207.1
   Greenbelt, Maryland 20771
   Reference: B73-10181

Patent status:

NASA has decided not to apply for a patent.

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