

**A VERSATILE SOFTWARE CONTROL SYSTEM  
FOR A TRIPLE QUADRUPOLE MASS SPECTROMETER**

C. A. Myerholtz, A. J. Schubert, M. J. Kristo and C. G. Enke

Department of Chemistry  
Michigan State University  
East Lansing, Michigan 48824

The complete computerization of a triple quadrupole mass spectrometer (TQMS) in our laboratory has been accomplished by a software control system that allows the operator to conveniently and flexibly control the instrument's 30 parameters and 5 different scan modes. FORTH has allowed us to create such a system by allowing the system programmers to tailor-make a command syntax specific to our application, while still allowing access to the FORTH kernel and application primitives.

The triple quadrupole mass spectrometer is a type of tandem mass spectrometer that was invented in our laboratory by Yost and Enke (1). The TQMS instrument consists of two quadrupole mass filters that are separated by a quadrupole collision chamber. In the TQMS experiment, the sample to be analyzed is first ionized in the source region. The resulting ions are then selected, according to their mass, in the first quadrupole mass filter. Ions having the mass selected by the first mass filter are then fragmented by collisions with a target gas in the collision chamber. The collision chamber is a quadrupole that is not mass selective. The first and third quadrupoles can be mass selective or not. The ions resulting from the fragmentation in the collision chamber can then be analyzed by the third quadrupole mass filter and detected by a continuous dynode electron multiplier. The TQMS has proved to be useful in direct mixture analysis and the determination of the structure of organic molecules (2,3).

A control system for the TQMS must have the following features: The system must have the ability to control the large number of controllable parameters. It must handle the full dynamic range of the ion current (  $10^8$  ). The system must reduce the large rate and volume of data collected in the experiment, which eventually must be stored on disk, by performing peak-finding in real-time. There should be facilities to display the raw ion signal in real-time and to display the acquired data during or by the end of the experiment. ( A display of the raw ion signal helps the user to optimize the different instrumental parameters. The display of the acquired data permits the operator to determine if the control system is operating properly and to monitor the course of an experiment. ) The system must be able to manage the data that the system acquires. Finally, the control system should be able to be mastered by mass spectroscopists and provide an environment for them to program complex experimental sequences. The following paragraphs give a brief description of how each of these

design goals was achieved with appropriate hardware and the FORTH programming environment.

One can set or change instrument parameters by entering them into the parameter editor, which is a screen-oriented menu, or by using the SET command. A set of "softknobs," which give the familiar feel of an analog dial with the convenience of digital control are also provided. These "softknobs" are optical rotary encoders that generate two streams of digital pulses upon rotation. From these two pulse streams, one can determine the direction and degree of rotation. The "softknobs" have no limit to their rotation. The shaft can rotate in either direction indefinitely. Since the action of the "softknobs" is controlled by software, the software can interpret the 250 pulses generated from each revolution of the dial in any way necessary. Thus, the "softknobs" can act as variable resolution devices. For instance, one could assign a full-scale change for 10 revolutions or increase the resolution ten-fold by assigning a full-scale change for 100 revolutions. The limiting resolution, then, is the resolution of the digital-to-analog converter. Non-linear or cyclical functions can be assigned to a knob with the appropriate software. "Softknobs" are connected to the master processor through an interface that converts the two input pulse streams to direction bits and a strobe signal. The strobe signal is used to interrupt the master processor each time a knob's position is changed. The processor can then read the direction bits to determine whether to increment or decrement a variable assigned to a device. These devices are a very satisfying way to adjust parameters that affect instrument output in real-time, as in "tuning-up."

The user can display acquired data in three ways. First, a DLIST command lists the data acquired from the last scan, or any selected scan, as a table of values for the scanned parameter and ion intensity. Secondly, the user can graphically display the acquired data as a mass spectrum or as a parameter sweep, whichever is appropriate. The software control system allows one to scan any instrumental parameter, not just mass. The resulting plot of ion intensity versus the parameter value is called a sweep. Both sweeps and mass spectra can be displayed linearly or logarithmically by the graphics display. These graphic displays allows the user to examine the data during the course of an experiment. Extensive interactive capabilities for the graphics are not provided, since that function is more appropriate for the host computer to which the data is eventually uploaded. Thirdly, raw ion current signal (without peak-finding) is sent to an oscilloscope in real-time. Thus, the user can immediately observe the effect of changing instrumental parameters. A digital-to-analog converter controls the x-axis. The computer also controls the gain of the amplifier which supplies the ion current signal to the y-axis of the oscilloscope. A split screen utility is also provided, which allows the user to display between one and five mass windows on the oscilloscope screen. The gain for each screen can be controlled separately. A split screen editor is provided for interactive control of the split screen task. This split screen function allows the user to see peaks which are widely separated in mass simultaneously. This is an invaluable aid in tuning the instrument.

The data from each scan is written to one of two Winchester Disks

for permanent storage, using polyFORTH database management. This facilitates easy storage and retrieval from the disk. Records of instrumental parameters and experimental notes, as well as the actual ion intensity data, are stored in variable-record scans. Scans are grouped into experiments and experiments are grouped into files. Eventually, all data are uploaded to an 11-23 minicomputer for archival storage and final analysis. The capabilities of the larger computer are better suited for constructing large databases and carrying out complex number crunching.

The software control system also allows one to define new commands easily. The user can define new experiments or experimental protocols to more effectively control the instrument. One can enter commands singly, all at once on a single line or by defining and invoking a new word. Each user can define a new method or utility to aid in his experiment. For example, one user defined an experiment that comprised 3700 scans. In the experiment, he investigated the effect of varying certain parameters, such as pressure in the collision chamber and the energy of the collisions, on ion intensity and transmission. He took several scans for each unique combination of values of the parameters of interest. The entire experiment took slightly over four hours, most of which the user spent in analyzing the data as it was collected. The experiment duplicated similar work which had been done previously on a different instrument having a lesser degree of computer control. The previous experiment had taken nearly two weeks of work. Thus, the new software control system saved the user an immense amount of time and effort. Most people use the control system to acquire a group of scans of various types, displaying the data immediately after collection. From the results of these scans, they can decide on the future course of the experiment. Again, the software control system minimizes the amount of time that the user spends on actual data collection and maximizes the time that he spends on data analysis and controlling the course of the experiment.

In conclusion, the software control system that we have written for the TQMS allows the user to take easy advantage of the high level of computer control of the instrument. The user has access to the inner workings of the computer and the instrument, while still having the higher-level application-specific words. The user can extend the command level by defining new words to perform useful functions. Programmers working with the system have readily extended its functions (such as to accommodate chromatography/mass spectrometry). Non-programmer mass spectroscopists have been able to easily utilize all programmed functions and combine them into completely automated, complex experiments.

## References

1. R. A. Yost, C. G. Enke, D. C. McGilvery, D. Smith, J. D. Morrison, Int. Journal of Mass Spectrometry and Ion Physics, 30, 1979, 127.
2. R. A. Yost and C. G. Enke, Analytical Chemistry, 51, 1979, 1251A.
3. R. A. Yost and C. G. Enke, Organic Mass Spectrometry, 16, 1981, 171.

