PREPRINT UCRL- 78347

CONF-760524-3

Lawrence Livermore Laboratory

COMPUTERIZED MASS SPECTROMETER DATA SYSTEM AT LLL

R. D. Friesen and R. J. Dupzyk

June 30, 1976

MASTER

American Society for Mass Spectrometry
May 9-14, 1976, San Diego.

COMPUTERIZED MASS SPECTROMETER DATA SYSTEM AT LLL*

R. D. Friesen, R. J. Dupzyk

Lawrence Livermore Laboratory, University of Cal 'ornia
Livermore, California 94550

ABSTRACT

The data systems on the three mass spectrometers at LLL are computer-controlled, pulse-counting systems synchronized to a repeatedly-swept magnetic field. The data are accumulated in the memory of the computer or in a Nuclear Data ND 180 in a multi-scaler mode of operation This mode of data acquisition allows a continuous check of the background stability and makes tune-up easier. But the main benefit is a reduction in the required ion emission rate stability. By the use of standards to set the system dead time, we have been able to utilize the sensitivity of a pulse counting system without the expense of exotic equipment.

Pulse Counting Equipment

The electron multiplier is an 18-stage EMI 9642/2B beryllium-copper venetian blind type. The socket is a specially made ceramic unit that forms the vacuum seal and electrical interface. Every stage is bypassed directly to ground. The first dynode is run at -3.5 to -6.0 kV (depending on the age of the multiplier). The last dynode, at ground potential, is dc coupled to the preamp.

Using an oscilloscope, the dead time of the multiplier was found to be 20 ns.

The preamplifier is an in-house design using a Fairchild 733 wide-band video amplifier. It is connected as a gain of 100 and performs the discrimination function also.

*Work performed under the auspices of the U.S. Energy Research & Development Administration under contract No. W-7405-Eng-48.

Using a fast double pulse generator, the measured dead time of the preamplifier was 13 ns.

The data counter was designed and built at LLL. It is a 100 MHz T^2L binary counter with switch selectable serial or parallel output. The serial output is used when the counter is connected to a Nuclear Data ND 180 and the parallel output is interfaced directly to the PDP-8. The counter's measured dead time is 10 ns.

The equation for combining the individual time components is:

$$DT = (M^2 + P^2 + C^2)^{1/2}$$

From this the system dead time should have been 25.8 ns.

To check our calculations, we ran several N.B.S. Uranium standards. We varied the emission rate over a .1% to 10.0% dead time correction range and adjusted the dead time correction until the isotope ratios remained constant over the entire range. The actual system dead time was approximately 40 ns. It varied with discriminator setting, multiplier voltage and the age of the multiplier.

Mode of Operation

Our instruments use a fixed high voltage and a swept magnetic field. The sweep is a linear ramp moving first up then down through the isotopic region of interest. The sweep times vary with sample requirements, but the average times are .25 to .5 seconds and the run times are 100 to 1000 seconds. Sweeping up and down through the spectrum tends to cancel long term emission drifts and repetitive sweeping improves the signal-to-noise ratio.

Computer System

The computer system CPU is a Digital Equipment Corporation PDP-8 with 16K of core. Bulk storage for the system is two Diablo disk drives, one fixed platter and one removable platter. Peripherals on the system are a 2400 baud Telray 3300 CRT terminal, a 100 character-per-second Centronics 306 printer, a 14 inch H-P 1300A display scope, a DEC high-speed paper-tape reader-punch, and an in-house fabricated joystick for operator data interaction.

The software for the system uses DEC's OS8/Λ3. The actual programs are written in FORTRAN II with assembly language subroutines for data acquisition, display, and control.

The system operation code is actually many small codes divided into levels and linked through a process called chaining. At the start, the code asks if this sample is an old or new type. If it is old, it uses a parameter file from a library. If it is a new type, the code asks questions until it has created a new parameter file which is then added to the library.

The parameter file sets the route through the nest of programs, it sets the type of data reduction, and it sets the data output format.

The nest of programs is divided into six basic levels of operation:

The first level establishes the initial parameters such as log number, sample identification, mass range, and system dead time. It also opens the variable file.

The second level does the data acquisition, either by reading the ND 180 memory or reading the data counter. When the data counter is being used, the program provides a linear or log display of the data as it accumulates. The program then writes the data into a temporary data file on the disk.

The third level allows the operator to correct any dropped channels or noise spikes that may have occurred. It then does data smoothing by an algorithm called a moving average. It then goes through the data a peak at a time, finding peaks and backgrounds. The computer's choice is displayed using cursors to mark the selected points. The operator may correct these choices and the program then calculates the peak heights and isotope ratios. These ratios and their errors are then printed. If the operator wishes to take more data, the chain goes back to the second level. If he is through, the chain goes on to the fourth level.

The fourth level calculates and prints the final ratios and errors from all the data accumulated. Then, depending on the experimental requirements, any further required calculations are performed.

The fifth level in the set gathers all the temporary data files into one permanent data file for long term storage and deletes all the the temporary files.

The sixth level retrieves the permanent data files and creates new temporary data files, allowing the data to be reprocessed if needed.

Results

The on-line computer and pulse counting system has allowed us to increase our precision and dynamic range. We are now reporting the following results:

For routine samples in the 50 picogram to 300 nanogram range, a precision of ± .5% on minor isotopes is obtainable. By special request (and handling) we have been able to report ± 10% precision on 10^8 atoms of sample, ± .2% precision on 1500-to-1 adjacent mass dynamic range, or ± 10% precision on 10^7-to-1 adjacent mass dynamic range.

cm