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CONTROL OF THE UTI 100C QUADRUPOLE MASS SPECTROMETER WITH AN IN--ETC(U)
SEP 82 D DAMLAREN, J ARNOLD, J C HEMMINGER

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Control of the UTI 100C Quadrupole Mass Spectrometer
with an Inexpensive Microcomputer

by

David Dahlgren, John Arnold, and John C. Hemminger

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Control of the UTI 100C Quadrupole Mass Spectrometer with an
Inexpensive Microcomputer

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Abstract

The interfacing of a UTI 100C quadrupole mass spectrometer to an inexpensive microcomputer system (the Commodore 32K Pet) is described. The system is capable of selecting and monitoring up to 13 masses simultaneously (on a time scale of one second). An example is given of the utilization of this system in the temperature programmed decomposition of dimethyltetrazine on a platinum surface.



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Introduction:

The typical control electronics for a quadrupole mass spectrometer provides a consecutive mass scan over a preset range. Many experiments are more appropriately designed to monitor the intensity of a certain mass or masses while an experimental parameter is varied. Standard control electronics allow one to carry out such experiments one mass at a time. An example of such an experiment is the thermal desorption experiment which has become a standard tool of surface science. In this experiment a molecule is adsorbed on the surface of interest. The surface is then heated rapidly and the intensity of the mass of interest is monitored as a function of surface temperature. The single mass detection capability of most control electronics in such experiments is not a problem when the molecule of interest is a simple one such as CO. In such a case monitoring mass 28 gives the data of interest. However, when more complex molecules or reactive systems involving several species are studied it is imperative that one be able to monitor several masses over a short time span (short compared to the time scale of the experimentally varied parameter). Several modern quadrupole mass spectrometers are now provided with more sophisticated control electronics which jump from one preset mass to the next and allow effective monitoring of several masses simultaneously. The major drawback of such systems is the expense and inflexibility of the additional electronics console which provides this function.

In this article we describe the interfacing of the control electronics for a UTI 100C Quadrupole Mass Spectrometer to a low cost microcomputer system, the 32K Commodore Pet. With this configuration we are able to monitor 13 masses per second at the same sensitivity, or 8 masses per second with different preset sensitivities for each mass. In addition we can simultaneously monitor the externally controlled experimental variable (in our experiments the sample temperature).

Hardware:

The control electronics for the UTI 100C quadrupole mass spectrometer are extremely well designed for easy interfacing to a computer system. Selection of the desired mass in the range 1 to 300 AMU is obtained with a voltage input of 0 to 10 volts. The sensitivity of the electrometer in the control electronics is controlled by shorting to ground the proper combination of four 32 volt reed relays. These relays are easily accessible at the rear of the control unit.

The computer we have utilized is the 32K Commodore Pet. the Pet has been interfaced to two 12 bit digital to analog converters for voltage output and two 32 bit frequency counters for signal input. Experimental voltages are read by the computer by voltage to frequency conversion followed by reading the frequency with one of the counters. This interface is controlled by an 8255A microprocessor which links to the 32K Pet through the memory-expansion port.¹ This allows direct access to the address and data bus. The Pet therefore sees the interface as memory locations. Further interfacing is accomplished via the Pet J-2 user port. The J-2 port consists of eight lines which are memory accessed with read/write programming of the computer logic level.²

Mass Selection:

As indicated above the standard UTI 100C control electronics make external mass selection straightforward. A d.c. voltage between 0 and 10 volts input to the control electronics provides mass selection in the range of 1 to 300 AMU. Thus the required voltage for consecutive masses differs on average by 33 millivolts. We use one of the 12 bit D/A converters to provide the voltage for mass selection. This provides us with a voltage resolution of ~ 2.4 millivolts. We have found that the voltage required for a particular mass can not be predicted with sufficient accuracy by assuming a simple linear relationship. Thus we predetermine the voltage required for a particular mass. This voltage appears to be extremely stable and once determined can be used with confidence. The 2.4 millivolt resolution we have with the 12 bit D/A converters gives us sufficient accuracy to jump directly to the peak of the desired mass. We normally carry out experiments with a mass spectrometer resolution which gives at least baseline resolution between neighboring masses up to 250 AMU. With this resolution a change of ± 2.4 millivolt in the mass selecting voltage causes a change of less than 5% in the intensity measured.

Output Signal Measurement:

The UTI 100C utilizes a channeltron electron multiplier as the ion detector. When the standard control unit is utilized the

output of the electron multiplier is measured with an electrometer which is an integral part of the control electronics. We read the signal level by reading the analog voltage output of the electrometer (0-10 volts). As we described above this is accomplished by voltage to frequency conversion (0-100 KHz) followed by frequency counting. It would be possible to read the signal out of the channeltron in a pulse counting mode with the counter. However, by continuing to utilize the electrometer it is extremely easy to switch back and forth from computer control to normal operation. Under normal operating conditions we obtain good signal to noise levels with 40 msec counting times for each mass.

The sensitivity of the electrometer is also easily switched externally as described above by shorting to ground the proper combination of four 32 volt relays which are accessible at the rear of the control unit. This is accomplished through the J-2 port. Shorting of the 32 volt relay is through a transistor (2N3053) which is turned on with the 5 volt computer logic level. There is also a hex, buffer driver with open collector (SN7407) between the computer J-2 port and the transistor for computer safeguard. We have found that a 50 msec delay following sensitivity change is required. A general schematic of the computer interface setup is shown in Figure 1.

Software:

The Commodore 32K Pet has a Basic interpreter and all programming associated with the mass spectrometer interfacing could

be done in Basic. However, the Pet is also easily programmed in machine language. The present version of our software utilizes machine language for all input/output, except the slower electrometer sensitivity control. All other manipulations are carried out via Basic. Once the data is obtained data manipulation may be carried out including output to a CRT, cassette tape or plotted on a line printer for hardcopy.

Discussion:

The system designed and programmed as described here is currently being used in temperature programmed thermal desorption studies. In our thermal desorption studies, gases are first exposed to a clean metal surface under ultra high vacuum conditions. After adsorption (usually at room temperature or below) has taken place the metal is resistively heated and the products desorbing from the surface are monitored as a function of temperature. The temperature of the sample is monitored by a chromel/alumel thermocouple spot welded directly to the crystal. There are two analog signals which must be digitized, read and stored by the computer. One is the signal from the thermocouple the second is the mass spectrometer signal. The thermocouple voltage is read, after amplification, by voltage to frequency conversion followed by frequency counting.

Utilizing the system we have described we can monitor the intensity of 13 masses and the sample temperature with a cycle time of one second if all the masses can be observed at the same electrometer sensitivity. When different sensitivities are utilized for different masses we can monitor 8 masses and the sample temperature with a one second cycle time.

Example:

An example of the mass spectral analysis of the thermal decomposition of dimethyltetrazine adsorbed on Pt(111) is shown in Figure 2.

H_2 , N_2 , HCN, and C_2N_2 are all major products of this reaction. With the present system we can easily monitor all these products and their cracking fragments simultaneously as shown in Figure 2. All types of data manipulation, such as smoothing, integration, background subtraction, scaling, etc. can be carried out easily.

Conclusion:

We have described a method of interfacing a UTI 100C Quadrupole Mass Spectrometer to an inexpensive microcomputer system, the Commodore 32K Pet. This allows us to monitor up to 13 masses effectively simultaneously (on a time scale of ~ 1 second).

Acknowledgements:

This work was supported in part by the Office of Naval Research, and the Hooker Chemical Corporation Grant of Research Corporation.

References:

1. This interface was constructed for us by Steve Smiriga of the University of California, Berkeley, Chemistry Department, Electronics Shop.
2. CBM User Manual, P/N 320856-3, Commodore Business Machines, Inc., 1979.

Figure Captions

Figure 1: General schematic of interfacing between UTI 100 C Control electronics and the Commodore 32K Pet.

Figure 2: Temperature programmed decomposition of dimethyltetrazine on Pt(111). Heating rate is 10 °C/sec.

- a) H₂ signal as mass 2.
- b) HCN signal as mass 27.
- c) N₂ signal as mass 28.
- d) C₂N₂ signal as mass 52.

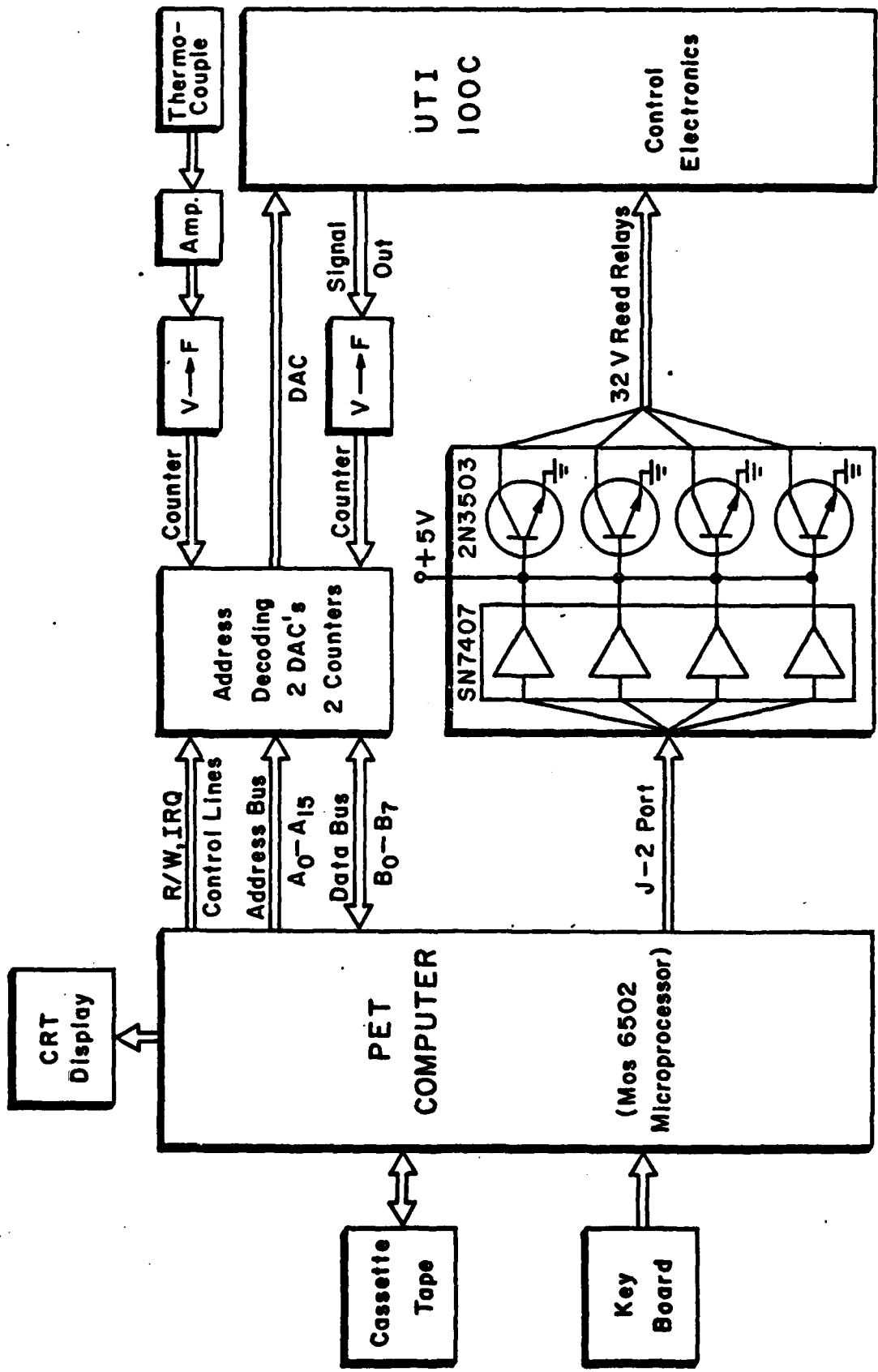


Figure 1

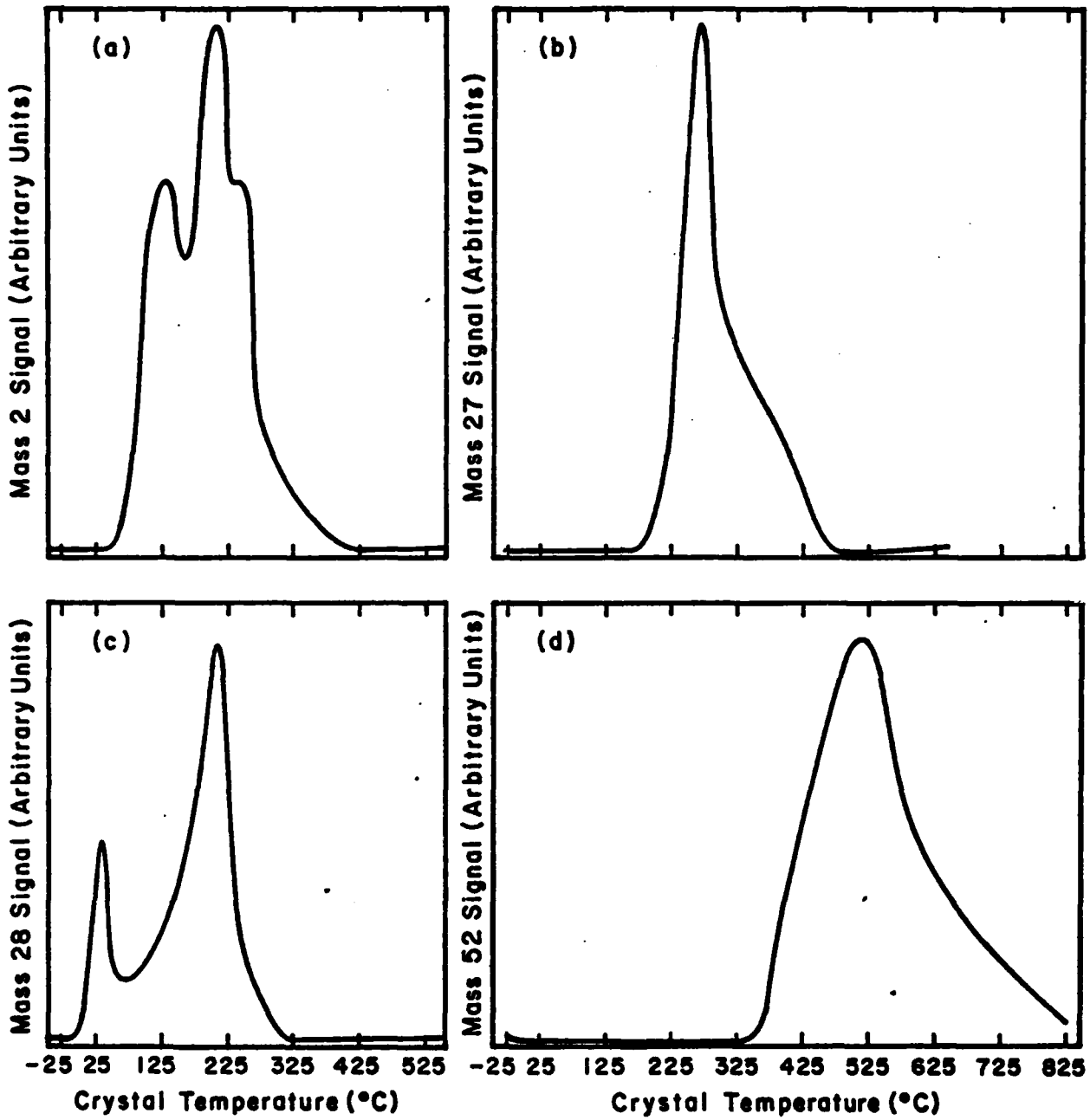


Figure 2

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