Identification and Quantitative Measurements of Chemical Species by Mass Spectrometry

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IDENTIFICATION AND QUANTITATIVE MEASUREMENTS 
OF CHEMICAL SPECIES BY MASS SPECTROMETRY 

Final 
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1. Background 

Mass spectrometry is often known as the gold standard of analytical chemistry techniques. No other method can provide a similar combination of general utility, response time, and detection sensitivity. But, mass spectrometers have typically been large, heavy, and required large amounts of power to operate. 

In 1999, Southwest Sciences began working with Mass Sensors (St. Louis, MO) to develop a miniaturized version of a double-focusing type of mass spectrometer. Much of that work was supported by NASA’s SBIR program. The analyzer portion of the Mass Sensors device – which was, in turn, based on intellectual property licensed from the University of Minnesota – is small enough to fit in the palm of one hand. It uses a combined magnetic and electrostatic fields to generate mass spectra; the magnetic field acts as a momentum selector (which is actually a mass analyzer) while the electrostatic field acts as an energy analyzer. Careful selection of the relative strengths of the two types of fields improves mass resolution by reducing the effects of the distribution of the ion kinetic energies. Although double-focusing mass spectrometers had been known for nearly 50 years, the key innovation in the Mass Sensors instrument was a novel method for constructing the elements used to generate the electrostatic field that nearly eliminated field distortion at the sides of the mass analyzer. This made it possible to shrink the analyzer so that ion trajectories filled nearly the entire open portion of the analyzer. Previous designs required the analyzer to be substantially large than the ion path cross section in order to guarantee uniform fields along the ion trajectories. 

The SBIR-funded work at Southwest Sciences showed the instrument to operate well at ion masses from about 15 to 110 daltons. The mass spectral peaks had a Gaussian shape with a fixed \( \frac{m}{\Delta m} \) width that allowed straightforward deconvolution of overlapping mass peaks. The mass spectrometer was equipped with a newly designed ion multiplier (Detector Technologies, Inc.) that allowed operation at sample pressures up to \( 10^4 \) torr, or an order of magnitude larger than is possible with conventional ion multipliers. This higher pressure operation further increased detection sensitivity by increasing the number density of analyte gas in the ion source region.
The initial success of Southwest Sciences’ work with the Mass Sensors mass spectrometer motivated the current project. A number of NASA programs – particularly space-borne and microgravity drop tower experiments – would benefit from the availability of a compact, truly portable, mass spectrometer. Potential applications ranged from monitoring crew physiology on board the ISS by measuring gases in exhaled breath to detecting reaction intermediates during microgravity combustion. Despite the successes of the SBIR-funded work, Mass Sensors was unable to commercialize their mass spectrometer technology. Nearly all of the instruments suffered from performance degradation – diminished ion signals, reduced mass resolution, or both – on a time scale ranging from several hours to several days. This problem was attributed to deposition onto the inner surface of the mass analyzer of pyrolysis products formed at the hot wire filament in the ionizer. Performance could be restored by cleaning the analyzer, but the problem would recur on the same short time scale. In some ways, the biggest unresolved question was why the instrument that was used at Southwest Sciences in the Phase II SBIR project performed as well as it did for such an extended time.

Given their inability to produce reliable commercial instruments, Mass Sensors was unable to bring products to market and, ultimately, terminated their business in February 2004.

When it became clear that Mass Sensors would not be able to meet the requirements of this project, Southwest Sciences turned to other sources of miniature mass spectrometers. Several vendors were offering devices intended, for the most part, as benchtop analytic instruments and used quadrupole, time-of-flight, or ion trap technology. We selected the quadrupole mass spectrometer manufactured by Ferran Scientific (San Diego, CA). Ferran’s technology was truly innovative. The mass analyzer consists of a 4 × 4 array of quadrupole rods that form a set of 9 (a 3 × 3 array) matched quadrupole filters operated in unison. The filter sits between a single ionization source and Faraday cup detector that serve all nine quadrupole sections. The entire assembly – ion source, quadrupole array, and Faraday cup – fits within a 12 cm³ vacuum enclosure. An electronics head, attached to the vacuum enclosure, measures 4.7 × 6.0 × 5.6 cm and weighs 100 g. The electronics base unit (computer network interface or CNI in Ferran’s syntax) is 5.9 × 14.0 × 16.1 cm, weighs 750 gm, and requires 1.5 A at 24 V DC.

We selected the Ferran device over other newly developed quadrupole mass spectrometers (such as the Stanford Research and Infinicon instruments) because the Ferran is smaller, can operate at higher pressures, and uses less power. Similar concerns – particular the operating pressure and electronics – helped rule out the ion traps and time-of-flight mass spectrometers. As mass spectrometers get smaller, vacuum requirements become more important because the size, weight, and power needs of the vacuum pumps exceed those of the mass spectrometers. For example, the miniaturized cylindrical ion trap mass spectrometer developed by Prof. Graham Cooks at Purdue University is roughly 1 cm³, but the entire instrument including pumps, electronics, and computer weighs 16 kg.¹ Much of the weight is due to the vacuum requirements.

2. Physical Description of the Delivered System

The completed mass spectrometer system is a fully-contained, automated instrument consisting of a needle sampling inlet, a custom-designed, small-scale gas chromatograph and a miniature, quadrupole mass spectrometer. The system is mounted on a two-tier, anodized aluminum breadboard having overall dimensions 38×45.5×30.5 cm, Figs. 1 and 2. The upper tier supports the sample control valves, chromatograph, mass spectrometer and controller, and turbomolecular pump. There is also space for a lecture bottle of helium to be used as the chromatograph carrier gas. The bottom tier contains a roughing pump and control electronics for the sampling inlet, chromatograph heater, multiport valve, and turbomolecular pump. A laptop computer that controls the instrument and collects data is also included.

The instrument operates using 120 VAC. Two uninterruptible power supplies (UPS) are included so that the user has a choice between operating time and UPS size and weight.

Figure 1. Photograph of the experimental setup. The top plate contains the sampling system (column, needle, valves) and turbomolecular pump while the lower plate contains the electronics, controllers, and diaphragm pump. The entire assembly plugs into one 120 V AC outlet.

Figure 2 - Photograph of the upper platform of the system showing the mass spectrometer, vacuum system, and gas chromatograph. There is room also for a carrier gas lecture bottle.
3. Operation of the Delivered System

3.1 Mass Spectrometer

The Ferran Scientific Symphony quadrupole mass spectrometer, billed by the vendor as “the world’s smallest mass spectrometer,” consists of three components. The micropole array (MPA) is the actual mass spectrometer that sits inside the vacuum system. It is a miniature array of quadrupole mass spectrometers designed to operate simultaneously (in parallel). Atoms and molecules are ionized in a single Nier-type ion source following electron impact (EI). Electrons are emitted from hot filaments located outside the field of view (main axis) of the quadrupole detector. Using electrostatic lenses, ions are extracted, focused, and injected into individual quadrupole mass filters. Ions with a specific mass-to-charge ratio are filtered by applying a combination of DC and RF voltages of the poles forming a quadrupole of the array. Filtered ions in each quadrupole are collected on individual Faraday type detectors. All individual detectors contribute to generate a single current signal. A mass spectrum is generated by scanning both AC and DC voltages applied on the poles of the Micropole. The MPA chassis includes a total of 16 rods and 11 electrical pins all secured in a glass-to-metal structure and sealed in a high temperature oven. Operation at high temperature avoids the type of contamination that plagued the Mass Sensors design.

The electrostatic lenses, apertures, and plates are made of photo-etched parts. The sensor construction does not use ceramic parts to avoid the type of patch charging effects that are common with other quadrupole mass spectrometers.

The Ferran quadrupole can operate at one of two ionization settings: 70 eV and 43 eV. All of the development work was done using 70 eV ionization.

The second part of the Ferran mass spectrometer is the spectra converter (SC), the blue box that attaches to the MPA and is shown in Fig. 3. The SC includes a pre-tuned RF power supply and an electrometer. Using a built-in guide pin, the SC is easily connected and secured to the back of the MPA with a connector latch. The combination can be mounted in any orientation. Ferran offers three different sizes of MPA and three different spectra converters. Specifications for the allowed combinations of the micropoles and spectra converters are listed in Table 1. The combination used in the deliverable is highlighted; it was selected to give the best combination of mass range and resolution.

![Figure 3 - Detail photograph of the spectra converter (SC) on the Ferran Scientific quadrupole mass spectrometer.](image)
The third portion of the mass spectrometer, the Computer Network Interface (CNI), Fig. 4, includes the power supplies, the control circuitry and the communications board. All circuits are driven by an internal microcomputer and embedded control software (firmware). The CNI connects to a PC via RS-232, RS-485, or TCP/IP serial interface, and to the SC using a shielded cable. The CNI (and the rest of the mass spectrometer) is powered by 24 V DC at up to 1.5 A.

An RS-232 serial interface is used in the deliverable for communication between the host laptop computer and the CNI. The settings are 9800 baud, 8 data bits, no parity, 1 stop bit, and XON/OFF flow control. Data strings are terminated by a line feed character (decimal 13). Communications with the CNI entail reading and/or writing a set of registers.

<table>
<thead>
<tr>
<th>MPA</th>
<th>MPA6-1-2/45</th>
<th>MPA6-11-2/45</th>
<th>MPA6-5-2/6</th>
<th>MPA6-7-2/65</th>
<th><strong>MPA6-5-2/100</strong></th>
<th>MPA6-1-4/300</th>
</tr>
</thead>
<tbody>
<tr>
<td>SC</td>
<td>SC6-18</td>
<td>SC6-18</td>
<td>SC6-14</td>
<td>SC6-14</td>
<td><strong>SC6-11</strong></td>
<td>SC6-07</td>
</tr>
<tr>
<td>mass range</td>
<td>2-45</td>
<td>2 - 45</td>
<td>2 - 65</td>
<td>2 - 65</td>
<td><strong>2 - 100</strong></td>
<td>4 - 300</td>
</tr>
<tr>
<td>resolution (FWHM)</td>
<td>0.5</td>
<td>1.5</td>
<td>0.8</td>
<td>0.9</td>
<td><strong>1.0</strong></td>
<td>1.5</td>
</tr>
<tr>
<td>$p_{\text{max}}$ (torr)</td>
<td>$1 \times 10^{-3}$</td>
<td>$1 \times 10^{-2}$</td>
<td>$5 \times 10^{-3}$</td>
<td>$7 \times 10^{-3}$</td>
<td><strong>$5 \times 10^{-3}$</strong></td>
<td>$1 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

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**Table 1 - Ferran Scientific Quadrupole Mass Spectrometers**

**Figure 4 - Computer Network Interface (CNI) for the Ferran Scientific quadrupole mass spectrometer.**
3.2 Gas Chromatograph

The custom gas chromatograph uses a micropacked, HayeSepQ, Silcosteel® column from Restek (2 m long × 1 mm i.d. × 1.59 mm o.d.). Silcosteel columns are composed of stainless steel on the outside but contain an inner coating of silica. The silica coating results in fewer adsorption problems relative to a stainless steel surface. The stainless steel exterior provides more rigidity and prevents column breakage, traits particularly desirable for drop tower and space-borne environments. The Silcosteel column contains 100/120 mesh adsorbents of HayeSepQ, an adsorbent that shows excellent separation for many organic species. The fine mesh allows for a large number of theoretical plates, thereby allowing greater separation of species eluting from the column. We have also used zero dead volume fittings where possible. Figure 5 shows chromatographs of mixtures of alkanes (top) and alkenes (bottom) in helium.

![Figure 5 - Chromatograms of 1000 ppm calibration mixtures of alkanes (top) and alkenes (bottom) in helium.](image)

The column is wrapped with thin (0.20 mm diameter), polyimide-insulated nichrome wire. By passing a current through the nichrome wire, the column can be resistively heated in a fast manner. The total resistance of the wire used to wrap the column is 452 Ohms, and thus currents of 0.25 A are used. The column is supported 3 cm above the top plate by three wires attached to posts. A fan was placed 12 cm directly above the center of the column for efficient and uniform cooling. Figure 6 shows a plot of the temperature response for warming the

![Figure 6 - Response of the column temperature to rapid warming and cooling.](image)
column from ambient temperatures to 155 °C starting at 70 s. The initial heating rate is ~ 90°C min⁻¹.

The low thermal mass of the wire also allows for rapid cooling. At 410 s the heating stops, the
fan is started, and an exponential temperature decay is observed with a time constant of ~ 40 s.
Cooling the column to near ambient temperatures occurs within three minutes. Overall, the duty
cycle due to heating and cooling of the column is ~ 10 minutes.

The column heater control and temperature monitoring are performed by a pair of PID
controllers (Omega CNi3222-C24). Two controllers are used because readout of the current
temperature is not possible during programmed temperature ramp. Hence, the second controller
simply provides a measurement of the instantaneous temperature.

Gas sampling and introduction to the chromatographic column are controlled by a pair of
commercial, computer-driven valves, Fig. 7. Samples are drawn through a needle into a small
reservoir using a three-port PEEK valve. The valve normally connects the reservoir to the vacuum
pump so that the reservoir remains evacuated until a sample is acquired. Then, the valve switches
to admit gas through the sampling needle into the reservoir. Flow rates for typical sample durations
are limited by the conductance of the needle. PEEK was chosen because of its excellent chemical
and thermal stability†. We found PEEK valves to leak under vacuum; but this is not a problem for
the sample inlet that is pumped continuously. In this case, the chemical properties of the valve are
more important than its vacuum characteristics.

**a) preparation**

mini-MS

![Diagram](Figure 7 - Computer controlled valves used for sampling acquisition and for injecting the
sampled gas onto the chromatographic column.)

**b) analysis**

mini-MS

A ten-port, two-position, stainless steel and Nitronic 60 valve from Valco (P/N ET2C10UWT)
is composed of stainless steel, has ten ports for 1/16" tubing, and is used to direct the sample from
the reservoir to the chromatographic column. The valve is controlled by a 24 V DC microelectric
actuator that can be switched by a 5 V logic signal from the computer. The valve can withstand up
to 300 psi gas pressure and temperatures up to 330°C. The bores inside the valve are the same size

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†See the Victrex web site: [http://www.victrex.com/](http://www.victrex.com/).
(0.75 mm) as the inner diameter of the tubing leading to the ports, thereby minimizing the amount of dead volume in the sampling regime. Although not all ten ports are needed for the current instrument design, the availability of additional ports for only a slight increase in cost allows for greater adaptability in future applications as well as for redundancy if any of the ports become unusable in the future.

3.3 Vacuum System

The delivered mass spectrometer system is equipped with a Pfeiffer Vacuum model TPD 011 turbomolecular pump backed by a Pfeiffer MVP 015-2 diaphragm pump. The turbomolecular pump and controller are visible in the photograph in Fig. 2. The pump is one of a new generation of small, lightweight turbo pumps, and has a nominal pumping speed of 10 liters sec⁻¹ for N₂ and 6 liters sec⁻¹ for He with an ultimate pressure of better than 5 × 10⁻⁵ mbar (4 × 10⁻⁵ torr). It can tolerate a backing pressure of up to 25 mbar (19 torr). Compression ratios are 3 × 10⁶ and 3 × 10³ for N₂ and He, respectively. The pump requires 1 A at 12 V DC and needs no external cooling. It weighs 1.8 kg.

One end of the diaphragm pump is visible in the photograph in Fig. 2. Rough outer dimensions for the MVP 015-2 diaphragm pump are 29 × 17 × 17 cm. The pump weighs 6.5 kg, draws 1.1 A at 120 V AC (60 Hz), has a nominal pumping speed of 1.1 m³ hour⁻¹ at 60 Hz, and can achieve an ultimate pressure of 4 mbar (3 torr), or a factor of 6 better than required for the TPD 011 turbomolecular pump.

3.4 Software

The delivered instrument is operated by a program, LabMPA-final written in LabVIEW that controls a sampling valve to acquire the analyte, transfers the sample onto the gas chromatograph column, ramps the column temperature, measures the mass spectral ion intensities at a series of user-defined peaks, and records the data to disk in ASCII format.

Communication between LabMPA-final running on the laptop computer and the mass spectrometer system uses a PCMCIA plug-in card that contains a pair of RS-232 serial ports. This brings to three the total number of serial ports. The computer’s built-in port (COM1) provides communication with the Ferran Scientific mass spectrometer’s computer network interface (CNI). The two ports on the PCMCIA card (COM4 and COM5) address a pair of PID temperature controllers (Omega model CNI322-C24). One regulates the GC column temperature and the other reports the instantaneous temperature back to the laptop. The program also accesses a National Instruments DAQCard-DIO-24 PCMCIA plug-in card that uses 0 to 5 V logic signals to control the two valves and the column cooling fan.

Figure 8 shows the user interface that appears when the program is first opened. The major user controls appear on the left-hand side of the panel. At the top, masses to scan, is the list of ion masses that are acquired during each measurement. The next five items control the timing of the sampling and gc operation. The last of the group, set point, is the target maximum temperature achieved by the chromatograph. We identify this value as a “target” temperature, because the upper bound is
constrained by thermal loss to the surroundings and so is affected by ambient air temperature, humidity, and air currents.

The central region of the panel, dominated by the chromatogram plot area, provides the measurement results as acquired including the actual column temperature, the most recently acquired ion signals (in torr partial pressure), and the elapsed time in seconds.

The right-hand region is used primarily for debugging and to help the user examine raw signals between the host computer and the Ferran controller.

Figure 9, shows the six major controls from the program main panel, and describes their use. This information is displayed graphically on a time line in Fig. 10. The setpoint temperature is a target value that, for

**Figure 8** - Front panel of the LabVIEW program used to control the mass spectrometer system and collect and store the chromatographic data.

**Figure 9** - Detail of program front panel showing the key timing and temperature controls.
temperatures ≥190 °C, may be limited by the ambient air temperature, humidity, and air currents. We have found it useful to set a target above the maximum achievable temperature since this drives the PID temperature controller more strongly at the upper end of the temperature cycle and helps maintain a linear temperature ramp.

Experimental results are written to disk in ASCII format comma-delineated rows and columns. In all cases, the first column is the measurement time (relative to 0.0 at the start of the run), followed by the column temperature in °C. Then comes the partial pressures in torr for the selected ion signals. The temporal resolution is determined by the number of mass peaks measured because the Ferran computer network interface establishes a minimum dwell time of 0.6 seconds per mass peak. The text box below is a portion of a data set acquired when the instrument was being set up and demonstrated at NASA Glenn Research Center in August 2004. The demonstration used a calibration mixture of alkanes (1000 ppm each of methane, ethane, propane, n-butane, n-pentane, and n-hexane).

<table>
<thead>
<tr>
<th>time, temp, amu0028, amu0043, amu0057</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0586E+1, 2.6600E+1, 8.3660E-6, 7.6010E-7, 6.3700E-7</td>
</tr>
<tr>
<td>1.3979E+1, 2.6600E+1, 6.8930E-6, 7.5580E-7, 6.1260E-7</td>
</tr>
<tr>
<td>1.8120E+1, 2.6500E+1, 6.4640E-6, 7.4810E-7, 6.3390E-7</td>
</tr>
<tr>
<td>2.2302E+1, 2.6500E+1, 6.1880E-6, 7.4990E-7, 6.2860E-7</td>
</tr>
<tr>
<td>2.6548E+1, 2.6500E+1, 6.2140E-6, 7.4610E-7, 6.2650E-7</td>
</tr>
<tr>
<td>3.0242E+1, 2.6500E+1, 5.9070E-6, 7.4630E-7, 6.2370E-7</td>
</tr>
<tr>
<td>3.4475E+1, 2.6600E+1, 6.0410E-6, 7.2740E-7, 6.3020E-7</td>
</tr>
<tr>
<td>3.8620E+1, 2.6600E+1, 5.8840E-6, 7.4380E-7, 6.3960E-7</td>
</tr>
</tbody>
</table>

The full data set is shown graphically in Fig. 11. The large mass 28 background and the noise are due to some air contaminating the helium carrier gas.

The LabVIEW program LabMPA-final automatically saves each chromatogram to disk using an automatically generated filename AUTOSAVE_nnnn.TXT where nnnn is a number beginning with 00000 that is incremented to prevent duplicating files. The user is given the opportunity to rename the autosaved file at the end of each run.
Figure 11 - Chromatographic and temperature data from demonstration run.
Appendix A
LabVIEW source code
LabMPA-final.vi

C:\WPDocs\Contracts\C01-07 (NASA ITD mass spec)\ITDlaptop\Ferran_MPA.llb\ITD\LabMPA-final.vi

Last modified on 8/31/2004 at 2:08 PM
Printed on 12/20/2004 at 4:14 PM
Second part of initialization routine.

Initiate serial communications with Ferran, format the array of selected masses, and tell Ferran to get started.
**First part of initialization routine.**

Clear the string indicators, error cluster, and wait loop counter. Update "status of scan"
Here's the important stuff.

1. Construct the string arrays needed to program the Ferran and the gas collection/sampling system.
2. Loop repeatedly to collect data.

Here's the important stuff.

1. Construct the string arrays needed to program the Ferran and the gas collection/sampling system.
2. Loop repeatedly to collect data.

And done!

3. Halt the mass scan and turn off the mass spec filament.
4. Save data to disk in comma-delimited ASCII format.

Get measurement time, read temperature, and update label on STOP button.
Wait for Ferran to report having finished a mass scan
Key VI: Read and plot mass signals, set valves, set temperature.
End of the outer loop.
Update loop counter
STOP if user has pressed the stop button or on error, else continue.
DSB init communications and close all valves.vi

Set all valves off
The above sub-VI formulates write strings from the array of masses; input parameters are the array, the desired command string, the value to be written. In this case, it will make a string: “WP00xx,0001\r” where xx is the mass (array element) of interest.
Initialize parameters for MPA: 70 eV, fast mode.
The sub
VI to the below
right
formulates an
array of
command
strings from
the
array of

<table>
<thead>
<tr>
<th>Sample time (s)</th>
<th>Sample duration (s)</th>
<th>start trap heater</th>
<th>send to MS</th>
<th>ramp start</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Ramp time (s)</th>
<th>Soak time (s)</th>
<th>Setpoint</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

The sub
VI to the below
right
formulates an
array of
command
strings from
the
array of
Start scan

- VISA resource name
- VISA resource name(out)
- write statement output
- error out
- array write read
- error in (no error)

- 0
  - W10001,0001\r
  - RI0002\r
  - RI0001\r
  - RI1009\r
  - RT1004\r
  - RI1009\r
Initialize VISA: Inputs an appended array of string expressions to write and outputs the values. The number of bytes initially at the serial port is set to zero.
wait with error clusters.vi

milliseconds to wait

error in (no error)  error out
Use sequence structure to guarantee that time is measured first then temperature.
DSB clear buffer.vi
C:\WPDocs\Contracts\C01-07 (NASA ITD mass spec)\ITDlaptop\Ferran_MPA.llb\DSB clear buffer.vi
Last modified on 8/31/2004 at 2:08 PM
Printed on 12/20/2004 at 4:32 PM
Read the mass strings

VISA resource name (out) [1/3]
expected byte count [132]
old style? [T/F]
array write read
appended array statements [abc]
VISA resource name (in) [1/0]
Read masses [abc]
extracts the values from the strings
values [DBL]
error found? [T/F]
status [TF]
error out [TF]
error in (no error) [TF]
Apparently, the I0027 command is important, even though it was never set to a value of one (1) in the first place.

Makes a dialogue box of the result of the write command so the user can confirm that the filament is indeed off.

Filament status: on
Mode: idle
# filaments available: 2
DSB stop scan.vi
C:\WPDocs\Contracts\C01-07 (NASA ITD mass spec)\ITDlaptop\Ferran_MPA.lib\DSB stop scan.vi
Last modified on 8/31/2004 at 2:08 PM
Printed on 12/21/2004 at 9:40 AM
Make array of time, pressure

Pair the arrays of each mass reading to the time array

(X and Y arrays) Multi Plot
DSB generate autosave file name.vi
C:\WPDocs\Contracts\C01-07 (NASA ITD mass spec)\ITDlaptop\Ferran_MPA.lib\DSB generate autosave file name.vi
Last modified on 8/31/2004 at 2:08 PM
Printed on 12/21/2004 at 9:42 AM
This VI first saves the data to disk in a comma-delimited ASCII format. The file is written after a file name is generated automatically using the default naming convention of AUTOSAVE_nnnnn.TXT where nnnnn starts at 0 and is incremented for each successive new file.

The user is prompted to rename the file, if desired. Note that the renaming consists of copying AUTOSAVE_nnnnn.TXT to the new name (or path) and then deleting the starting file.

If no action is taken, the auto-saved file remains on disk until it is manually deleted or moved by the user using Windows tools.
This VI writes a setpoint temperature to the Omega temperature controller in COM5 (default).
DSB rename saved data file.vi
C:\WPDocs\Contracts\C01-07 (NASA ITD mass spec)\ITDlaptop\Ferran_MPA.lib\DSB rename saved data file.vi
Last modified on 10/29/2004 at 1:54 PM
Printed on 12/21/2004 at 9:46 AM
Appendix B
Ferran Scientific communications protocols
Programming Reference

Introduction

Programming the System is accomplished by writing to registers in the CNI (or CNI) module. These registers are organized into banks of registers. The current values of various registers can be read by performing Read requests. Likewise, the current values of various registers can be changed by performing Write requests.

Here is a summary of the five banks and their general functions.

<table>
<thead>
<tr>
<th>Bank Letter</th>
<th>Bank Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>AMU Pressure</td>
<td>The AMU pressure bank stores the current partial pressures measured for each AMU.</td>
</tr>
<tr>
<td>P</td>
<td>AMU Priority</td>
<td>Stores numbers which express the relative priority of each AMU. Setting values in this bank allows increasing or decreasing the System’s response time to various AMU’s.</td>
</tr>
<tr>
<td>I</td>
<td>Integer Status</td>
<td>Stores all System status and control registers that are best expressed as nonfractional numbers.</td>
</tr>
<tr>
<td>N</td>
<td>Analog Pressures</td>
<td>Stores each data point collected during the last AMU scan. It is the information from this bank that gets accumulated and processed into the results seen in Bank A. WARNING: Obtaining information from this bank requires a magnitude more RS-232 (or RS-485) communications between the Master and the System. Reading information from this bank is not recommended unless it is completely necessary.</td>
</tr>
<tr>
<td>R</td>
<td>Real Status</td>
<td>Stores all System status and control registers that are best expressed as numbers in scientific notation.</td>
</tr>
<tr>
<td>T</td>
<td>Text Status</td>
<td>Stores all alphanumeric information. For example, the System’s model number and serial number can be read from this bank. In addition, this back stores the current error message.</td>
</tr>
</tbody>
</table>

The details of each of these banks are described later. The next section describes the protocol used to read and write information into these banks.
Format of the Packets

This section covers the general format for all communication between the System and a Master. There is only one difference in protocol between CNI Module's operating in RS-485 mode versus RS-232 mode: The network mode requires transmitting characters in 9 bits instead of the normal RS-232 mode of 8 bits. This difference is also discussed in the following section.

Send Packets

There are two types of packets to send to the System: a Read Request and a Write Request packet.

Read Request:

\texttt{RL####[:AAAA][:Comment}{CR}}

Write Request:

\texttt{WL####,DATA[:AAAA][:Comment}{CR}}

where:

- \texttt{L} is replaced by a character which stands for the desired bank:
  - \texttt{A} AMU Pressure bank
  - \texttt{P} AMU Priority Control bank
  - \texttt{I} Integer Status/Control bank
  - \texttt{R} Real Status/Control bank
  - \texttt{T} Text Status bank

- \texttt{####} The number of the register to read or write within the bank selected. Remember that all numbers must be right justified.

- \texttt{:AAAA} An optional parameter which can be used as a packet sequence number. Each letter A stands for an ASCII letter or number. If the Master uses this option in a command, the System will send back a colon (:) followed by the exact four characters that it received. In effect, this can act as a packet sequence number that the Master can use to manage packets received.

- \texttt{;Comment} An optional parameter which both sides can use to contain comments. In general, the comment should not be used by either side because it lowers communications speed. If register I0005 is set to 1, then the System will include comments for all errors.

- \texttt{,DATA} A parameter that contains the information to write into the bank. Note that each bank stores a specific type of information: Integer (4 digit integer), Real (\#.###E+-##), or Text (ASCII text).
Receive Packets
There are two types of packets that a Master can receive: an Error packet and an Answer packet.

Error packet:

\[ EL###,\text{eeee[:AAAA]}[;\text{Comment}]{\text{CR}} \]

Answer packet:

\[ AL###,\text{Response[:AAAA]}{\text{CR}} \]

where:

\[ \text{eeee} \quad \text{The error number.} \]

\[ \text{L####} \quad \text{The bank and register where the operation occurred.} \]

\[ ;\text{Comment} \quad \text{A brief error message. By default, the System doesn't send error messages. But, setting the register I0005 to 1 will enable error messages to be placed in this area. Please see the information on I0005 in the Details of Banks section for more information.} \]

\[ \text{,Response} \quad \text{A reading of the register read or written. Normal responses are #### for integer variables, and #.###E+## for real numbers.} \]

**NOTE:** After the System performs a write, it will send a response in the same format as a response to a read. This allows the external program to confirm that the correct write took place.

Protocol of the CNI Module when in RS-485 mode
This section discusses the difference between the normal RS-232 mode and the RS-485 mode of the Computer Network Interface Module.

Four-Wire RS-485 Cable
The System CNI Modules use a four wire RS-485 cable. Two of the wires are transmutation lines from the Master. The other two wires are transmission lines from all of the CNI's that are on the cable.

Token-Type Protocol
To allow several CNI's to transmit on the same communications lines, a "token"-type protocol was established. In this protocol, all CNI's on the lines listen for a special address character that identifies to which CNI the Master is communicating. When a CNI receives its address, it automatically turns on its RS-485 transmitter and begins to listen for any commands that are
placed on the network. At the same time, all other CNI's disable their transmitters and continue to wait for the special address character.

9-Bit Serial Protocol

To help speed this process and to minimize interruptions to CNI's that are not part of the current "conversation", a 9 bit serial protocol was adopted. In this protocol, the UART of the Master (and the UARTS of all of the CNI's) enable a special 9 bit serial mode. (As opposed to a normal 8 bit serial mode.) In this mode, the normal 8 bits are transmitted plus an extra bit that the programmer can switch. This extra bit is used to mark whether a character is a special address character or a normal one.

Special vs. Normal Characters

When a 9 bit character's ninth bit is set to a 1, all CNI's use the other 8 bits as an address. When the 9th bit is set to a 0, the remaining 8 bits are read normally. For example, here is a sample message that the Master may send to the network lines:

\[
\begin{align*}
\text{2WI0001,0001\{CR}\} & \quad \text{'Tell CNI at 2 to turn on scan mode} \\
\text{AI0001,0001\{CR}\} & \quad \text{'CNI at address 2 responds}
\end{align*}
\]

The number 2 (that is in bold) is the only character that is sent with its ninth bit set. This command tells the CNI at address two (2) to turn on scan mode. The CNI that has its Configuration Switches set to address 2 will turn on its transmitter when it receives the 2. It will also receive the WI0001,0001 command and will respond. This CNI continues to keep its transmitter on and continues to receive and respond to commands sent by the Master to the network. The Master does not have to send the address character until it wants to address a different CNI.

In contrast, all other CNI's that receive the address 2 will turn off their transmitter (if they had it on), and will not receive or respond to the WI0001,0001 command. These CNI's will remain "dormant" until another special address character (a 9 bit character with the extra bit set) with their address is received.

**NOTE:** The word dormant refers to their transmitters being off. The CNI's will still continue to run normally in the mode that they were placed in. For instance, the Master could send the following sequence of packets:

\[
\begin{align*}
\text{2WI0001,0001\{CR}\} & \quad \text{'turn on scan mode for CNI at address 2} \\
\text{AI0001,0001\{CR}\} & \quad \text{'CNI 2 responds to the command} \\
\text{3WI0001,0000\{CR}\} & \quad \text{'"turn on" idle mode for CNI at address 3} \\
\text{AI0001,0000\{CR}\} & \quad \text{'CNI 3 responds to the command} \\
\text{4WI0001,0001\{CR\} } & \quad \text{'turn on scan mode for CNI at address 4} \\
\text{AI0001,0001\{CR\} } & \quad \text{'CNI 4 responds to the command}
\end{align*}
\]

The CNI that is at address 2 will turn on Scan Mode and will continue to run in Scan Mode even after the address 3 and address 4 are sent. Also note that the response packets from the CNI's are completely normal and do not include a network address. (They will be transmitted in 9 bits however.)
WARNING: If you set the Configuration switches so that two or more CNI's have the same address, they will all turn on their transmitters and garble each others' responses.

One final note, the Master should not send a new address to the network until a CNI has finished responding to its last given command. Doing so can cause the response to be garbled.

Details of the Banks

General Notes

All of the information that an external program needs to read or write is contained in a register of one of the banks. These sections detail what each of the registers control or report.

Before continuing, there are a few notes to point out about register numbers and reading from or writing to register numbers that don't exist.

- All register numbers are four digits long. Register numbers for some of the banks have their first digit coded. (The Integer, Real and Text banks are examples.) A 1 as the first digit means the register is READ ONLY. A zero or any other number means that it can be written to or read from. For example, bank T, the Text Status Bank, has a register 1001 that stores the manufacturer's name. This register, because its first digit is 1, is read only.

- When you read from or write to a register that doesn't exist, you will receive a communications error message. Depending on how you write your communications software, this can lead to a lock-up. As a short explanation, you may write software that unintentionally asks for an AMU that doesn't exist. The Micropole firmware will respond with a communications error. Your software may be designed to retransmit the packet if any communications errors occur. This, of course, causes the firmware to send the same communications error. This process could then repeat forever. You can write some error checking code to make sure that your software does not do this. See registers I1005 and I1006 for information on the System's capabilities.

AMU Pressure Bank (BANK A)

The AMU pressure bank stores the current partial pressure (in Torr) of each of the AMU’s the System has measured. The registers are read only. Register number one (1) corresponds to AMU number one (1). The System does not report partial pressures of fractional AMU’s. (See the Analog Pressure Bank for more information.)

General Format:

RA####{CR}

Example:

RA0040{CR} 'Read the partial pressure of AMU 40.
Read requests of an AMU number that is beyond the abilities of the analyzer will get a zero response or an error message. To help the external software, the minimum and maximum AMU's can be obtained by reading registers I1005 and I1006.

All registers in this bank default to 0.000E+00 Torr upon power up, reset or when the System is first changed to a non-idle mode.

**AMU Priority Bank (BANK P)**

This bank roughly controls the amount of time spent on each AMU that the MPA can measure. Each of the registers represents one AMU and contains an integer from 0 to 2. The System scans registers (AMU) with 2's twice as often as AMU’s marked with 1's. AMU's marked with 0 receive no scanning whatsoever.

You can increase the scan speed of the System significantly by setting the priority of the gases that you are not interested in with a 0.

Here are some examples:

- WP0040,0002(CR) 'Make AMU 40 a higher priority
- AP0040,0002(CR) 'AMU 40 now has priority 2.
- WP0006,0000(CR) 'Do not scan AMU 6
- AP0006,0000(CR) 'AMU 6 has priority 0 and won’t be scanned

This bank defaults to values of 1 when the System is powered up or reset. You can change the values of all of the registers in this bank with a single write to register I0020. Please see the appropriate section for more information.

**Integer Status Bank (BANK I)**

This bank controls the various options of the System. It also contains information that is most conveniently stored as an integer. The power up and reset values of the register are indicated with the word default in parentheses.

<table>
<thead>
<tr>
<th>Register Number</th>
<th>Name</th>
<th>Description/Value</th>
</tr>
</thead>
</table>
| 10001           | Device Mode     | 0 = Idle (default)  
1=Scan Mode (continuous)  
2=Leak Detection Mode  
3=Calibration Mode (not yet available)  
4=Scan and Hold Mode  
6=Jump Scan  
9999=Internal Test Mode. Used for factory testing of the CNI. DO NOT PUT THE SYSTEM INTO THIS MODE: System can be |
<table>
<thead>
<tr>
<th>Register Number</th>
<th>Name</th>
<th>Description/Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>10002</td>
<td>Reset Device</td>
<td>0=No (default) 1=Perform full reset. All registers are returned to their power-up defaults</td>
</tr>
<tr>
<td>10003</td>
<td>Degas Mode</td>
<td>0=Degas Off (default) 1=Degas On. e Energy Mode and the filament emission is turned to High.</td>
</tr>
<tr>
<td>10004</td>
<td>Electron Energy Mode</td>
<td>0=Low, 42V (default) 1=High, 68V (Not Available)</td>
</tr>
<tr>
<td>10005</td>
<td>Verbose Error Messages</td>
<td>0=No error message text sent. (default) 1=All error messages will be followed by text describing the error. NOTE: You can get the error message text by reading the T1005 or T1007 register.</td>
</tr>
<tr>
<td>10006</td>
<td>Auto Range Mode</td>
<td>not used. Reserved for future</td>
</tr>
<tr>
<td>10007</td>
<td>Leak Detection Gas</td>
<td>not used. Reserved for future</td>
</tr>
<tr>
<td>10008</td>
<td>Calibration Gas</td>
<td>not used. Reserved for future</td>
</tr>
<tr>
<td>10009</td>
<td>Automatic Shutoff Period</td>
<td>0=Automatic shutoff deactivated. (default) Any other number written here activates the automatic shutoff. If you read this register, it will return the number of minutes left before shutoff.</td>
</tr>
<tr>
<td>10010</td>
<td>Continue Scan</td>
<td>1=Put In Hold 0=Release From Hold (default) Used only with Scan Once and Hold. After every scan, the System sets this register to a one (1). The System doesn't begin another scan until a zero (0) is written here by the Master.</td>
</tr>
<tr>
<td>10012</td>
<td>Electrometer Speed Select</td>
<td>not used. Reserved for future</td>
</tr>
<tr>
<td>10013</td>
<td>Range switch Speed select</td>
<td>not used. Reserved for future</td>
</tr>
<tr>
<td>10014</td>
<td>AMU Cal Speed select</td>
<td>1 = Fast; 1 = Medium; 5 = Slow; 10 = VSlow</td>
</tr>
<tr>
<td>10015</td>
<td>Analyzer EmissM</td>
<td>This is a MPA calibration factor. It should not be changed from the value that the factory has given.</td>
</tr>
<tr>
<td>10016</td>
<td>Autozero mode</td>
<td>0=enabled 1=disabled not used. Reserved for future</td>
</tr>
<tr>
<td>10017</td>
<td>Start scanning at AMU</td>
<td>0=Start scanning at the minimum AMU the System can measure (default) A non-user number is treated as the first AMU to measure in a scan.</td>
</tr>
<tr>
<td>10018</td>
<td>End scanning at AMU</td>
<td>0=End scanning at the maximum AMU the System can measure (default) A non-zero number is treated as the last AMU to measure in a scan.</td>
</tr>
<tr>
<td>10019</td>
<td>Total Pressure Mode</td>
<td>0=off (default) 1=on</td>
</tr>
<tr>
<td>10020</td>
<td>Set Priority Bank</td>
<td>Sets the priority bank to the value written here.</td>
</tr>
<tr>
<td>10021</td>
<td>Version</td>
<td>Acceptable power level 6, 7, 8, and 9 (no check)</td>
</tr>
<tr>
<td>10022</td>
<td>CNL I/O</td>
<td>Logic Function Enabler</td>
</tr>
<tr>
<td>10023</td>
<td>Force</td>
<td>0=Automatic (default); 1=Filament A; 2=Filament B</td>
</tr>
</tbody>
</table>
# Chart of Bank I Registers

<table>
<thead>
<tr>
<th>Register Number</th>
<th>Name</th>
<th>Description/Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>10024</td>
<td>Filament # of Samples for OSC mode</td>
<td></td>
</tr>
<tr>
<td>10025</td>
<td>Mux Position for OSC mode</td>
<td></td>
</tr>
<tr>
<td>10026</td>
<td>User Specified # of points / AMU</td>
<td></td>
</tr>
<tr>
<td>10027</td>
<td>Hold Filament ON</td>
<td>0=off (default) 1=on</td>
</tr>
<tr>
<td>10028</td>
<td>Hold More Point Scanning</td>
<td>0=Fast; 1=Medium, Slow, VSlow</td>
</tr>
<tr>
<td>10029</td>
<td>Dwell Time</td>
<td>Reserved for future.</td>
</tr>
<tr>
<td>10030</td>
<td>E. Multiplier</td>
<td>Reserved for future.</td>
</tr>
<tr>
<td>10031</td>
<td>Load NOVRAM</td>
<td>Reserved for future.</td>
</tr>
<tr>
<td>10032</td>
<td>Low Gain Mode</td>
<td>Lock Electrometer in VFast Scan. Reserved for future.</td>
</tr>
</tbody>
</table>

## Read Only Registers

<table>
<thead>
<tr>
<th>Register Number</th>
<th>Name</th>
<th>Description/Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>11001</td>
<td>Error Code</td>
<td>0=No errors occurred. (default) Any other number represents an error. See the section on Error Codes for more information. The text of this error is stored in register T1005.</td>
</tr>
<tr>
<td>11002</td>
<td>Scan Time</td>
<td>not used. Reserved for future.</td>
</tr>
<tr>
<td>11003</td>
<td>Scan Counter</td>
<td>This register counts the number of scans that have occurred. This gets updated at the end of each scan and can be used to tell when a scan has been completed</td>
</tr>
<tr>
<td>11004</td>
<td>Last AMU Processed</td>
<td>not used. Reserved for future.</td>
</tr>
<tr>
<td>11005</td>
<td>Lowest AMU</td>
<td>Lowest AMU that the System can measure using the SC and MPA connected. WARNING: This register is valid only when an SC is connected to the CNI or CNI. (Defaults to 0 if no SC connected.)</td>
</tr>
<tr>
<td>11006</td>
<td>Highest AMU</td>
<td>Highest AMU that the analyzer can measure using the SC and MPA connected. WARNING: This register is valid only when an SC is connected to the CNI or CNI. (Defaults to 0 if no SC connected.)</td>
</tr>
<tr>
<td>11007</td>
<td>Maximum Number of Filaments</td>
<td>Total number of filaments on the MPA.</td>
</tr>
<tr>
<td>11008</td>
<td>Number of Usable Filaments</td>
<td>Number of filaments on MPA that are available for use.</td>
</tr>
<tr>
<td>11009</td>
<td>Filament</td>
<td>0=All filaments are off 1=Filament A is in use 2=Filament B is in use</td>
</tr>
<tr>
<td>Register</td>
<td>Name</td>
<td>Description/Value</td>
</tr>
<tr>
<td>----------</td>
<td>------</td>
<td>-------------------</td>
</tr>
<tr>
<td>I1010</td>
<td>Status Number of Electrometer Ranges</td>
<td>Not used. Reserved for future.</td>
</tr>
<tr>
<td>I1011</td>
<td>Communications Error Code</td>
<td>0=No Errors. (default) Any other number represents an error code. See the section on Error codes for more information. The text of this error is stored in register T1007.</td>
</tr>
<tr>
<td>I1012</td>
<td>Pressure Threshold Trip Status</td>
<td>No used. Reserved for future. See R0004 for more information.</td>
</tr>
<tr>
<td>I1013</td>
<td>Current AMU Reading</td>
<td>This register stores the AMU numbers that are currently being scanned by the System.</td>
</tr>
<tr>
<td>I1014</td>
<td>SC Code</td>
<td>Resistor Code</td>
</tr>
</tbody>
</table>

**Real Status Bank (BANK R)**

This bank contains the various configuration options of the MPA. It also contains information that is most conveniently stored as a real number.

<table>
<thead>
<tr>
<th>Register Name</th>
<th>Name</th>
<th>Description/Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>R0001</td>
<td>Manometer Span, Volts/Torr</td>
<td>0=No manometer connected (default) A zero (0) written here means that the manometer will not be read or used for filament protection. Otherwise, the span of the manometer as expressed in Volts/Torr is stored here.</td>
</tr>
<tr>
<td>R0002</td>
<td>Manometer Zero Offset</td>
<td>0=No manometer zero offset (default) This stores the zero offset of the manometer, expressed in Torr. The System will then subtract this number from all readings of the manometer.</td>
</tr>
<tr>
<td>R0003</td>
<td>Pressure of Calibration Gas</td>
<td>Not Used. Reserved for future.</td>
</tr>
<tr>
<td>R0004</td>
<td>Threshold Trip Pressure</td>
<td>Not Used. Reserved for future.</td>
</tr>
<tr>
<td>R0005</td>
<td>Analyzer Sensitivity Factor Adjust</td>
<td>611 (default) The Sensitivity calibration factor provided by the factory for the Micropole Analyzer currently connected to the System.</td>
</tr>
<tr>
<td>R0006</td>
<td>Analyzer Ion Adjust</td>
<td>12 (default) The Analyzer ion calibration factor provided by the factory for the MPA currently connected to the System.</td>
</tr>
<tr>
<td>R0007</td>
<td>Analyzer AC Adjust</td>
<td>6.6 (default) The Analyzer AC calibration factor provided by the factory for the MPA currently connected to the System.</td>
</tr>
<tr>
<td>R0008</td>
<td>User Sensitivity Adjust</td>
<td>1.000 (default) A multiplier for sensitivity of the analyzer. If the System reports a Nitrogen peak of 1 mTorr when it should read 2 mTorr, a two (2) can be written here to adjust the reported sensitivity.</td>
</tr>
</tbody>
</table>
# CHART OF BANK R REGISTERS

<table>
<thead>
<tr>
<th>Register Name</th>
<th>Name</th>
<th>Description/Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>R0009</td>
<td>Analyzer</td>
<td>AMULOC 1.000 (default)</td>
</tr>
<tr>
<td></td>
<td>Description</td>
<td>The calibration factor provided by the factory for the Micropole currently</td>
</tr>
<tr>
<td></td>
<td>Value</td>
<td>connected to the System.</td>
</tr>
<tr>
<td>R0010</td>
<td>Analyzer</td>
<td>TSense Adjust 6000 (default)</td>
</tr>
<tr>
<td></td>
<td>Description</td>
<td>The calibration factor provided by the factory for he Micropole currently</td>
</tr>
<tr>
<td></td>
<td>Value</td>
<td>connected to the System.</td>
</tr>
<tr>
<td>R0011</td>
<td>Electron</td>
<td>Energy Reserved for future.</td>
</tr>
<tr>
<td>R0012</td>
<td>Calibration</td>
<td>Frequency Reserved for future.</td>
</tr>
</tbody>
</table>

## READ ONLY REGISTERS

<table>
<thead>
<tr>
<th>Register Name</th>
<th>Name</th>
<th>Description/Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1001</td>
<td>Total N2 Equiv Pressure</td>
<td>Reading The current reading of total pressure. Only updated when total pressure</td>
</tr>
<tr>
<td></td>
<td>Reading</td>
<td>mode is on. See 10019 for more information.</td>
</tr>
<tr>
<td>R1002</td>
<td>Manometer Reading</td>
<td>The current reading of the manometer, in Torr</td>
</tr>
<tr>
<td>R1003</td>
<td>Lowest Detectable Pressure</td>
<td>The lowest pressure the System can detect, in Torr.</td>
</tr>
<tr>
<td>R1004</td>
<td>Highest Detectable Pressure</td>
<td>The highest pressure the System can detect, in Torr.</td>
</tr>
<tr>
<td>R1005</td>
<td>Highest Pressure Before</td>
<td>Shutdown If the pressure exceeds this value, the System will turn off the filaments</td>
</tr>
<tr>
<td></td>
<td>Shutdown</td>
<td>and return to the idle mode.</td>
</tr>
<tr>
<td>R1006</td>
<td>SC Temperature (C)</td>
<td>Obsolete. Was used for CNI’s to report current temperature of the SC Module.</td>
</tr>
<tr>
<td>R1007</td>
<td>Max SC Temperature</td>
<td>Allowed Maximum rated temperature for the SC Module.</td>
</tr>
<tr>
<td></td>
<td>Allowed</td>
<td></td>
</tr>
<tr>
<td>R1008</td>
<td>Fil. A ON Time</td>
<td>0.1h Granularity</td>
</tr>
<tr>
<td>R1009</td>
<td>Fil. B ON Time</td>
<td>0.1h Granularity</td>
</tr>
</tbody>
</table>
Text Status Bank (BANK T)  
This bank stores information and messages about the System. It also contains information that is most conveniently stored as a text.

<table>
<thead>
<tr>
<th>Register Number</th>
<th>Name</th>
<th>Description/Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1001</td>
<td>Manufacturer’s Name</td>
<td>Contains the name of the factory that created the CNI Module.</td>
</tr>
<tr>
<td>T1002</td>
<td>CNI’s (or CNI’s) Model Number</td>
<td>Contains the CNI Modules’ model number.</td>
</tr>
<tr>
<td>T1003</td>
<td>Serial Number of CNI (or CNI)</td>
<td>Not Used. Reserved for future.</td>
</tr>
<tr>
<td>T1004</td>
<td>Firmware Version</td>
<td>Contains the Firmware version number.</td>
</tr>
<tr>
<td>T1005</td>
<td>Last Error Message</td>
<td>This will have the last error message. (Note: Communications errors are not recorded here.)</td>
</tr>
<tr>
<td>T1006</td>
<td>SC’s Model Number</td>
<td>Contains the model number of the SC that is currently connected to the CNI Module.</td>
</tr>
<tr>
<td>T1007</td>
<td>Last Communications Error</td>
<td>This will have the last communications error message.</td>
</tr>
<tr>
<td>T1008</td>
<td>SC S/N</td>
<td>Reserved for future.</td>
</tr>
<tr>
<td>T1009</td>
<td>MPA Model</td>
<td>Reserved for future.</td>
</tr>
<tr>
<td>T1010</td>
<td>MPA S/N</td>
<td>Reserved for future.</td>
</tr>
</tbody>
</table>

Analog Pressure Bank (BANK N)  
This bank stores the actual point-by-point readings of the System. The registers are read only and their contents are an (X,Y) pair of coordinates for the data point read. Unlike Bank A, the register number refers to the number of the data point and not the number of the atomic mass unit.

An (X,Y) pair that has X=0 marks the end of the data points for the scan run. Otherwise, the X value is the AMU number in the format of ###.#. The Y value is the partial pressure (in Torr) measured at the AMU X. Here is an example:

RN0001(CR)  
give me the data point number 1
AN0001,002.4,1.120E-03  
partial pressure read at AMU 2.4

To use this bank, you need to keep reading data points until you encounter one that has an X value of 0. For this reason, the length of the packet, and the number of data points in a typical scan, it is NOT recommended that you read this information. See the Optimization of Results section of this manual for more information.
Appendix C
Ferran Scientific data sheet
Symphony
Micropole™ Mass Spectrometer System

- Faster Scan Rates (600 ms / amu)
- $10^{-10}$ Torr Limit of Detection
- 10 parts per billion Sensitivity
- 43 eV or 70 eV Ionization Energy Settings
  - $2 \times 10^{-8}$ atm.cm$^3$/s Minimum Detectable He Leak Rate
- New PlasmaGuard Extends Sensor Life

FSInc. March - 2002
**Symphony** is the world’s smallest complete mass spectrometer system. The small size, low cost, and component interchangeability provide the user with a set of powerful features and unique advantages. The mix-and-match feature is crucial for easy upgrade, troubleshooting, and replacement. In addition, the ability to operate at higher pressures (mTorr range) without sacrificing UHV measurement capabilities translates into a two-fold advantage: measuring gaseous concentrations directly using an open source and reducing or eliminating additional vacuum pumps. Since the vacuum pumping requirements are less stringent, Symphony systems can be packaged together with various sample introduction methods in the form of portable instruments for field applications.

At the heart of the Symphony is an enhanced version of the Micropole™ (U.S. Patent 5,401,962) mass analyzer, the PlasmaGuard. Its breakthrough design using a miniature array of quadrupole mass filters revolutionized the world of mass spectrometry. The Micropole offers a similar or greater sensitivity than conventional mass spectrometers, but in a fraction of the volume. Its fabrication (U.S. Patent 5,857,890) uses cutting edge technologies such as highly accurate photo etched components and proprietary glass-to-metal seals. The mass production of these sensors translates into a lower manufacturing cost. Connected to the PlasmaGuard is a state-of-the-art miniature, low power, high frequency power supply. Since these units are factory pre-tuned, they are interchangeable. The sensors are pre-calibrated against transfer pressure standards in order to provide direct absolute total and partial pressure measurements (in Torr). Through a computer interface, the instrument is controlled using MS Windows compatible software (WinMPA). Automatic, around the clock data acquisition in different formats is built-in for fast access to the information required from the mass spectrometer.
Symphony Components:

Micropole and PlasmaGuard Analyzers:

The Micropole (MPA) is a miniature array of quadrupole mass spectrometers designed to operate simultaneously (in parallel). Atoms and molecules are ionized in a single Nier-type ion source following electron impact (EI). Electrons are emitted from hot filaments located outside the field of view (main axis) of the quadrupole detector. Using electrostatic lenses, ions are extracted, focused, and injected into individual quadrupole mass filters. Ions with a specific mass-to-charge ratio are filtered by applying a combination of DC and RF voltages to each quadrupole in the array. Filtered ions in each quadrupole are collected on individual Faraday type detectors. All individual detectors contribute to generate a single current signal. A mass spectrum is generated by scanning both AC and DC voltages. A MPA chassis includes a total of 16 rods and 11 electrical pins all secured in a glass-to-metal structure. The structure is sealed in a high temperature oven. The electrostatic lenses, apertures, and plates are made of highly accurate photo etched parts. The sensor construction does not use ceramic parts as is the case with conventional quadrupoles. Therefore, no charging effects are observed.

The Symphony system features a more robust version of the Micropole: the PlasmaGuard. It is encapsulated in a stainless steel case for easy handling. The analyzer is also protected by a mesh, on the vacuum fitting, designed to extend the lifetime of the sensor in harsh environments such as plasma processes. Each MPA/PlasmaGuard sensor is delivered with a set of six calibration parameters generated at the factory for fast and easy operation. Two ionization energy settings are built into the Symphony system: 70 eV and 43 eV. While 70 eV is standard, 43 eV setting is used to avoid spectral interferences from doubly charged ions. For example, the water peak at (m/e = 18 amu) is free from \(^{36}\text{Ar}^{++}\) interferences since, 43 eV is just below the second ionization potential of \(^{36}\text{Ar}\).

Spectra Converter (SC):

The SC includes a pre-tuned RF power supply and a extremely sensitive electrometer circuitry. Using a built-in guide pin, the SC is easily connected and secured to the back of the MPA/PlasmaGuard with a connector latch. The combination can be mounted in any orientation. MPAs/PlasmaGuards and SCs are interchangeable for fast and easy replacement, upgrade, and troubleshooting.

Computer Network Interface (CNI):

The SC is connected to the CNI using a shielded cable. The cable is immune against surrounding electronic noise from other equipment. The CNI includes the power supplies, the control circuitry and the communications board. All circuits are driven by an internal microcomputer and embedded control software (firmware). The CNI is directly connected to a PC via RS232, RS485, or TCP/IP serial interfaces. For multiple sensor installations, an RS232/RS485 converter is on board. The CNI is powered by a 24 VDC power supply.

Computer Network Logic Interface (CNL):

In addition to the CNI circuitry, the CNL includes a board with digital Input/Outputs and analog output capabilities. A standard Capacitance Diaphragm Gauge (CDG) connection is also available. The additional circuitry enables the user to implement fault detection scenarios using custom decisions based on the data acquired. Automatic operation using external triggers is easily set. Connecting a CDG or other equivalent gauge to the CNL to work in conjunction with the RGA allows the user to implement warning, automatic operation, and sensor protection features.
**Symphony Specifications:**

**Micropole and PlasmaGuard Analyzers (MPA and SMPA):**
- Dimensions: see drawing
- Weight: 100 g
- Twin-Filament Electron Impact Ion Source
- Filaments: Y2O3/Ir (standard), ThO2/Ir, W
- 9 miniature Quadrupole Mass Filters
- Mass Filters: 2, 5, 10, 15, 20 mm Long
- Faraday Cup Detector
- Max. Bake out Temperature: 350 °C
- Max. Operating Temperature: 150 °C
- UHV Compatible: < 10⁻⁹ atm.cm³/sec Rate
- Mounting Flange: mini-Conf (standard), NW/KF16

**Spectra Converter (SC):**
- Dimensions: see drawing
- Weight: 200 g
- RF Power Supplies: 7, 11, 14, or 18 MHz
- Factory Pre-Tuned
- Interchangeable with any MPA/SMPA Analyzer of the Same Type
- Connector Latch for Mounting in Any Orientation

**Computer Network Interface (CNI):**
- Dimensions: see drawing
- Weight: 750 g
- Power Requirements: 24 VDC, 1.5 A
- RS232 (15 ft Max.), RS485 (3000 ft Max.) Interfaces
- RS232/RS485 Converter
- Selectable Baud Rates: 9600, 19600, 38400
- Up to 8 Units can be Daisy-Chained
- Built-in standard connections to heated and non heated Capacitance Diaphragm Gauges (See **TRIO** Brochure)

**Computer Network Logic Interface (CNL):**
- Dimensions: see drawing
- Weight: 1 kg
- Power Requirements: 24 VDC, 1.5 A
- RS232 and RS485 Interfaces
- RS232/RS485 Converter
- Selectable Baud Rates: 9600, 19600, 38400
- Up to 8 Units can be Daisy-Chained
- 8 Open Collector Logic Input/Outputs
- Standard Connector for non Heated CDGs
- 2 Pneumatic Valve Actuators
- Optional 3 Analog Outputs (0-1V)

**Accessories (See Catalog/Price List for Part Numbers):**
- 24 VDC Power Supply (35 and 65 W)
- Micropole Cable (1, 10, 15, 25 ft max.)
- RS232 Cable (6, 10, 25, 50 ft Max.)
- RS485 Cable (1, 3000 ft Max.)
- RS232/RS485 Converter
- Isolation Valves (manual and Pneumatic)
- Flange Adapters and Mounting Kits
- Grounding Strap (3 ft max.)
**Symphony Options:**

<table>
<thead>
<tr>
<th>PlasmaGuard (SMPA)</th>
<th>Spectra Converter (SC)</th>
<th>Micropole Analyser (MPA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SMPA-1-2/45-X</td>
<td>SC6-18</td>
<td>MPA6-1-2/45-X</td>
</tr>
<tr>
<td>SMPA-5-2/45-X</td>
<td>SC6-14</td>
<td>MPA6-5-2/45-X</td>
</tr>
<tr>
<td>SMPA-7-2/45-X</td>
<td>SC6-14</td>
<td>MPA6-7-2/45-X</td>
</tr>
<tr>
<td>SMPA-5-2/100-X</td>
<td>SC6-11</td>
<td>MPA6-5-2/100-X</td>
</tr>
<tr>
<td>SMPA-1-4/300-X</td>
<td>SC6-07</td>
<td>MPA6-1-4/300-X</td>
</tr>
</tbody>
</table>

**Ordering Information:** A desired mass range requires specifying a combination of SMPA/SMPA and SC. Please contact the Sales department for prices and delivery.

1. (X) specifies the vacuum flange type: C for 1.33" Conflat and K for NW/KF16

**Total Process Monitoring and Control Solution**

- **SMPA-5-2/65C:** PlasmaGuard (5 mTorr Upper Pressure limit, 2-65 Amu mass range, mounted on mini Conflat Flange)
- **SC6-14:** 14 MHz Spectra Converter
- **CNL-06:** Computer Logic Interface
- **PS-03:** 24 VDC Power Supply
- **CA-06-X:** SMPA Shielded Cable
- **CA-02-YY:** RS232 Cable
- **Control Software (WinMPA2002)**
- **VG-1A (1 Torr CDG; See TRIOT Brochure)**
- **V12:** Optional Pneumatic valve

**Shipping Information:**

<table>
<thead>
<tr>
<th>Weight</th>
<th>Packaging Dimensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 kg Approx.</td>
<td>45x40x10 cm</td>
</tr>
</tbody>
</table>

XX: Cable Length = 6, 10, 15’
YY: Cable Length = 6, 10’

For turnkey solutions, please refer to the Quartet brochure available on Ferron.com. The Quartet system, AC line powered, includes a Symphony components, data display and control monitor.

For Miniature, low cost, reliable CDGs, please refer to the TRIO brochure available on Ferron.com.
WinMPA™ Control Software:

**Symphony** is controlled using WinMPA, a Windows application developed by Ferran Scientific Inc. In addition to the communication protocols, WinMPA includes data acquisition, display, and file handling capabilities. When executed for the first time, WinMPA performs a three-step configuration procedure. 1. **ANALYZER CONFIG.** consists of entering the calibration parameters of each MPA/SMPA. The parameters of the analyzer are stored under a name (e.g. serial number) specified under NEW ANALYZER. 2. **SYSTEM CONFIG.** a SYSTEM comprises a MPA/SMPA, a SC, and CNICLN. Under NEW SYSTEM, the model and the serial number of the SC and CNICLN are entered. The MPA/SMPA is selected from a pull-down menu showing all analyzers configured under ANALYZER CONFIG. 3. **COMM CONFIG.** consists of linking a SYSTEM to a communication port of the PC. After setting the baud rate, the serial interface (RS232 or RS485) is selected. For multiple sensor applications, each SYSTEM has an address (0 through 32). A SYSTEM STATUS window enables the user to control, open graphs, save data, and generate process recipes for each SYSTEM independently.

**WinMPA Highlights**

- Compatible with Windows XP, 2000, Me, NT 4.0, 95/98, 3.1/3.11
- PC Requirements: 66 MHz, 16 MB RAM. Higher specifications are required for multiple analyzer installations.
- Embedded demo mode
- Capture of all data all the time in temporary files
- Automatic 24/7 data capture and file naming
- Binary and ASCII data file formats
- Dynamic Data Exchange (DDE) links with spreadsheet software.
- Optional TCP/IP protocol
- Data display in multiple, simultaneous BAR, TREND, ANALOG, TABLE, and DEVIATION graphs.
- Torr, Pascal, Bar, and PPM Units.
- Linear and Logarithmic Scales
- LEDs to show status of Input/Outputs
- Monitor and display signals from complementary gauges such as CDGs.
- Custom warnings following drifts from set tolerances
- Storage of process control recipes.
- Statistical process control (SPC) incorporated into recipes
- Deviation graphs showing drifts from “ideal” runs
- Event-driven full automated operation and data storage
- Jump/Continuous Scans with or without Total Pressure measurement
- Pre-set scan speed mode and graph recipes
- Sensor accumulated hours of operation
- Helium leak mode with progressive display graph and audible warning
Symphony Typical Applications

General Residual Gas Analysis:
- Vacuum diagnosis from UHV to low vacuum
- Troubleshooting leaks
- Monitoring and control of contaminants
- Helium leak detection

Semiconductor Chip Manufacturing:
- Photore sist detection
- Moisture & contaminant detection in wafer handling chambers of cluster tools
- Wet clean recovery after PM cycles
- Leakback test and leak troubleshooting
- Process monitoring and control
- Tool diagnostics and characterization

Space Research:
- Hazardous gas detection
- Life support and leak detection onboard Space Station
- Planetary and moon Exploration: Mars, Europa

R&D:
- Multi-sensor deployment
- Remote operation
- Particle accelerators
- Synchrotrons

Industrial Vacuum Coating:
- Vacuum and optical coating
- Vacuum furnaces
- Glass coating
- Preventive maintenance
- Cryogenic pumps performance

Environmental Monitoring:
- Detection of volatile organic compounds (VOCs)
- Abatement monitoring
- Oceanography applications
Since it was founded in 1989, Ferran Scientific Inc. has established itself as the world leader in miniature, low cost pressure measurement and gas analysis. Using patented innovations in vacuum technology, Ferran Scientific Inc. was able to respond to pressing needs for affordable in-situ gas instrumentation. Upon its introduction, the Micropole mass spectrometer has enjoyed worldwide acceptance and success as one of the technological breakthroughs in 30 years of quadrupole mass filter designs. The Micropole continues to be a workhorse in affordable mass spectrometry with an impressive installed base in a variety of industries. The Micropole, in its newly released Symphony system, is the world’s smallest complete mass spectrometer system. These consumable sensor type instruments have provided lower cost of ownership in numerous applications. Using its expertise in miniaturization and mass production employing cutting edge technological tools, Ferran Scientific Inc. is able to manufacture instruments such as mass spectrometers and pressure gauges for a wide range of usage. The interchangeability of sensors and electronics adds an unprecedented plug-and-play concept for easy troubleshooting, upgrade, and replacement. The company’s turnkey solutions enable the user to minimize the installation time and rapidly extract gas pressure and analysis information.

**FERRAN SCIENTIFIC**

Affordable Gas Measurement, Control and Analysis

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U.S.A

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Fax: (858) 792-0065
E-mail: sales@ferran.com
Identification and Quantitative Measurements of Chemical Species by Mass Spectrometry

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51570 Pacheco Street, Suite E–11
Santa Fe, New Mexico 87505

National Aeronautics and Space Administration
Washington, DC 20546–0001


The development of a miniature gas chromatograph/mass spectrometer system for the measurement of chemical species of interest to combustion is described. The completed system is a fully-contained, automated instrument consisting of a sampling inlet, a small-scale gas chromatograph, a miniature, quadrupole mass spectrometer, vacuum pumps, and software. A pair of computer-driven valves controls the gas sampling and introduction to the chromatographic column. The column has a stainless steel exterior and a silica interior, and contains an adsorbent of divinylbenzene that is used to separate organic species. The detection system is based on a quadrupole mass spectrometer consisting of a micropole array, electrometer, and a computer interface. The vacuum system has two miniature pumps to maintain the low pressure needed for the mass spectrometer. A laptop computer uses custom software to control the entire system and collect the data. In a laboratory demonstration, the system separated calibration mixtures containing 1000 ppm of alkanes and alkenes.

The system is a fully-contained, automated instrument consisting of a sampling inlet, a small-scale gas chromatograph, a miniature, quadrupole mass spectrometer, vacuum pumps, and software. A pair of computer-driven valves controls the gas sampling and introduction to the chromatographic column. The column has a stainless steel exterior and a silica interior, and contains an adsorbent of divinylbenzene that is used to separate organic species. The detection system is based on a quadrupole mass spectrometer consisting of a micropole array, electrometer, and a computer interface. The vacuum system has two miniature pumps to maintain the low pressure needed for the mass spectrometer. A laptop computer uses custom software to control the entire system and collect the data. In a laboratory demonstration, the system separated calibration mixtures containing 1000 ppm of alkanes and alkenes.