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Design and Implementation of a Protection System for NMR Spectrometers

G. Laurent and M. Guéron[1]

Groupe de biophysique de l'UMR 7643 du CNRS, Ecole polytechnique, 91128 Palaiseau, France

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We have implemented a scheme, SPECMON, for monitoring various parameters of a spectrometer, such as nitrogen pressure and sample temperature, and taking corrective action. The scheme is based on considerations of protection management which are of general application. Evaluation of the spectrometer state is incorporated in macros of the application software (VNMR) and is therefore very flexible. In contrast, corrective action is limited to the single one which is deemed fully safe: complete shutdown of the spectrometer and logging. Shutdown is implemented by a minor hardware modification of the spectrometer: the introduction of a second input to a relay already present for protection of the spectrometer power supply. Monitoring is handled by the host computer, and the shutdown command is transmitted via control lines of its series port, independent of the standard connection between the host computer and the NMR system console. The monitoring system (software and hardware) is unobtrusive in normal conditions, and it can be tested without affecting the operation of the spectrometer. © 2002 Elsevier Science (USA)

Key Words: **flexibility; monitoring; protection; shutdown; spectrometer.**

INTRODUCTION

An NMR spectrometer often runs for long, unattended, periods, during which malfunctions may occur, with possibly severe consequences for the sample, the spectrometer, or the environment. Such malfunctions include an interruption of the nitrogen gas supply, a disconnection of a thermocouple or sample heater connector, or hardware or software failure of a radiofrequency or gradient pulse generator. These malfunctions could lead to overheating or freezing of the sample, to probe damage, or to damage to the electronics console. One should therefore attempt to automatically monitor emergencies and take corrective action.

If monitoring were perfect, one could design an array of responses to the different incidents. But perfect monitoring should not be expected, the more so since the incentive to refine monitoring is weak because malfunctions are rare. In this uncertain situation, the only sound corrective action is to attempt to put the spectrometer and sample in a safe state, sacrificing the experiment. We are thus led to the concept of a single, global response, and it must be appropriate for all conditions which require corrective action. We believe that the only response which can satisfy such requirements is complete shutdown, to be described below.

A protection system should be inconspicuous in normal conditions. Furthermore, it should not trigger unduly, whether in normal conditions or during incidents brought about by erroneous software or by unpredictable user actions. Nor should it be incapacitated by such incidents. In particular, cold or warm reboots should not trigger the protection response. Launching of a second version of the application hardware should not perturb the protection system. And unruly stops and starts should not lead to a situation where the inconspicuous protection system is in fact not running at all, a situation where the instrument would not only be insecure but would also be believed secure!

Such considerations have strong implications for the design of the protection system. In particular, special attention should be paid to initialization conditions and questions. The protection system itself should be designed to fail graciously if it fails. And physically disconnecting it, whether on purpose or not, should not affect spectrometer function. Similar concerns are found in the literature dealing with safety and control of nuclear reactors, space-based instruments, medical diagnostic equipment, etc. (*1, 2*).

In the present article, we present a monitoring and protection system, SPECMON, for a Varian Unity Inova 500-MHz high-resolution spectrometer. It consists of a combination of hardware and software such that the spectrometer can be shut down by a call to a submacro of the application software, VNMR. Thus, any condition which is detected or analyzed by the application software VNMR, or reported to it, can easily be used as a trigger for appropriate and logged spectrometer shutdown.

Beyond the description of this specific protection system, the article should hopefully prove useful for the conception and implementation of a protection system for spectrometers of other brands and other types, such as solid state spectrometers and clinical imagers.

Supplementary data for this article are available online.

[1] To whom correspondence should be addressed. E-mail: mg@pmc.polytechnique.fr.

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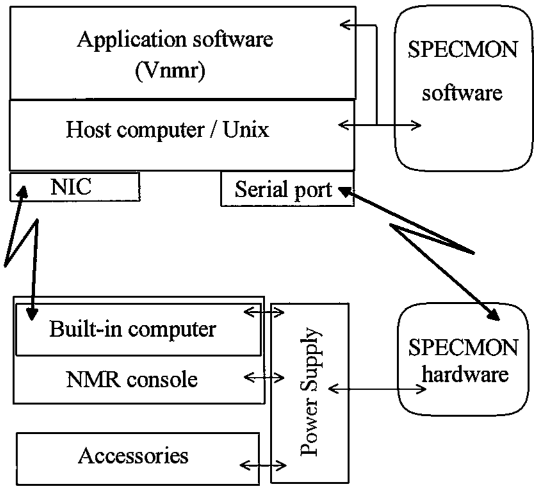

FIG. 1. General organization of the spectrometer (left side) and of SPECMON (right side). The spectrometer includes two parts: (top left) the host computer with its system software and NMR application software and (bottom left) the NMR console, with the built-in computer. The host computer communicates with the built-in computer of the NMR console via a network interface card (NIC) and cable. On the right are the two SPECMON components. Top right: the software is installed in the host computer. Bottom right: SPECMON hardware is housed in the NMR console. It communicates with the SPECMON software via a cable connected to a serial port of the host computer. It operates on the power supply of the NMR console.

GENERAL FEATURES OF THE PROTECTION SYSTEM

Figure 1 shows the general organization of the spectrometer (left side) and of SPECMON (right side). The spectrometer includes two parts. On the top left is the *host computer* with its system software and NMR application software. Below it is the *NMR console*, which houses the electronics for excitation and recording of the NMR signal and which includes a built-in computer. The spectrometer includes other components, for instance the magnet, which is not represented, and accessory equipment such as a cold-gas source. These other components are included if appropriate whenever the term "NMR console" is used. The host computer communicates with the built-in computer of the NMR console via a network interface card (NIC) and cable.

On the right are the two SPECMON components. The software (top right) is installed in the host computer. It is in communication with the system (Unix) and application (VNMR) software. SPECMON hardware (bottom right) is housed in the NMR console. It communicates with the SPECMON software via a cable connected to a serial port of the host computer. It can turn the power supply of the NMR console.

The goal that we set for SPECMON is to protect against failures of the spectrometer or of ancillary systems, with the exception of the host computer. The protective action is the same in all cases, a shutdown of spectrometer and ancillary systems, but not of the host computer. The decision to shut down is based on continuous evaluation of system parameters, most of which are to be read from the application software, VNMR.

The separation of the spectrometer into two parts, the non-monitored host computer and the rest, seems unavoidable. It leads us to distinguish between different types of failures.

1. Failures of the NMR console are properly handled by SPECMON. They do not affect the SPECMON software and signals, since these come directly from the host computer, and do not use the communication channel between the host computer and the NMR console. The SPECMON hardware is mostly independent of the NMR console, except that it uses one of its power supplies. This defect of principle could be easily remedied, but it is not worth the complication at this stage.

2. In normal conditions, the computer built in the VNMR console is responsible for running the experiment. From time to time the host computer performs read–writes on the built-in computer. The design of the spectrometer ensures that a failure of the host computer (alone) does not damage the VNMR console and does not interrupt the current experiment for some time. Failure of the host computer will disable SPECMON with no consequence, provided that SPECMON is built to react gracefully, so that as far as possible it does not trigger shutdown if the host computer fails or is rebooted or crashes.

3. A failure of both the host computer and the VNMR console is unmanageable by SPECMON, but it should be very rare. The single exception is that of a power failure affecting both parts. But such a failure does not create a specific problem, since it puts the VNMR console in the same state as a SPECMON-triggered shutdown.

IMPLEMENTATION OF SPECMON

The VNMR macro "specmon" includes a succession of *control routines*, each of which calls a submacro which handles the monitoring and evaluation of one instrument parameter, as provided to VNMR, primarily by the NMR console and possibly also by other sensors. For instance, one control routine could deal with nitrogen gas pressure, another with sample temperature, etc. In the case of a fragile sample, the temperature control routine could check for a deviation of "less than $+2°C$ from the programmed temperature during more than 1 minute," whereas, for a sturdy sample, a larger temperature deviation would be tolerated, etc. If shutdown is required, the submacro writes to the log file "/var/specmon/log" and calls the submacro "rs232_sh" for spectrometer shutdown.

This submacro shells out to a Unix program "rs232" which can read–write the specified RS232 serial port of the host computer (a Sun Ultra 1 of which we use port B). It sets two of the output control lines, RTS and DTR. These are connected to an operational amplifier (SPECMON hardware, Fig. 1) which triggers the relay, K201, of the Varian spectrometer power supply. The hardware modifications on the INOVA NMR console are minimal.

Three control routines are included in the specmon macro. The first is only for testing. The second handles the nitrogen gas pressure. The third is a model for implementing control of other parameters. All control routines are identical except for the section directly related to the controlled parameter. This section is easy to write and test since it is typically coded entirely in the framework of the application software and its macros. Timings, calls related to the shutdown procedure, tests of the serial port, etc. are already taken care of.

We present successively the situation in normal use, the spectrometer setup, the shutdown hardware, the program architecture, the present implementation, and suggestions for future work.

NORMAL USE

In normal use, starting VNMR will automatically start the specmon macro in active status, as a background task, as explained in the file `install.eng`. As long as no anomaly is detected, SPECMON remains invisible.

The Unix commands "`ps -ef | grep specmon`" or "`pgrep -fl specmon`" will show if the specmon macro is running. The program can also be switched to standby status (using the macro `sm_stand`) and it can be returned to active status with the macro `sm_activ`. When in standby, the specmon macro will print a line to screen every time it runs through its infinite "while" loop (default duration : 1 minute):

```
The SPECTROMETER MONITORING macro is
  DE-ACTIVATED Type 'sm_activ' to
  reactivate, or call the administrator.
```

SETTING UP THE SPECTROMETER

The spectrometer includes:

—a Sun Ultra 1 host computer with an Internet connection
—the NMR system console (the electronics cabinet), magnet, and probe
—a variable temperature accessory
—a nitrogen gas supply

Before considering any complementary protection measure, one should pay attention to the original (Varian) setup of the spectrometer and to its external supplies, primarily electricity but also nitrogen gas and possibly others.

The NMR console is powered via a master relay, K200 (Fig. 2). This relay disconnects in various conditions, including a power failure. Reconnection requires manual operation of the starter switch S200. Hence, in case of interruption of spectrometer function due to disconnection of K200, the NMR console will not restart on its own.

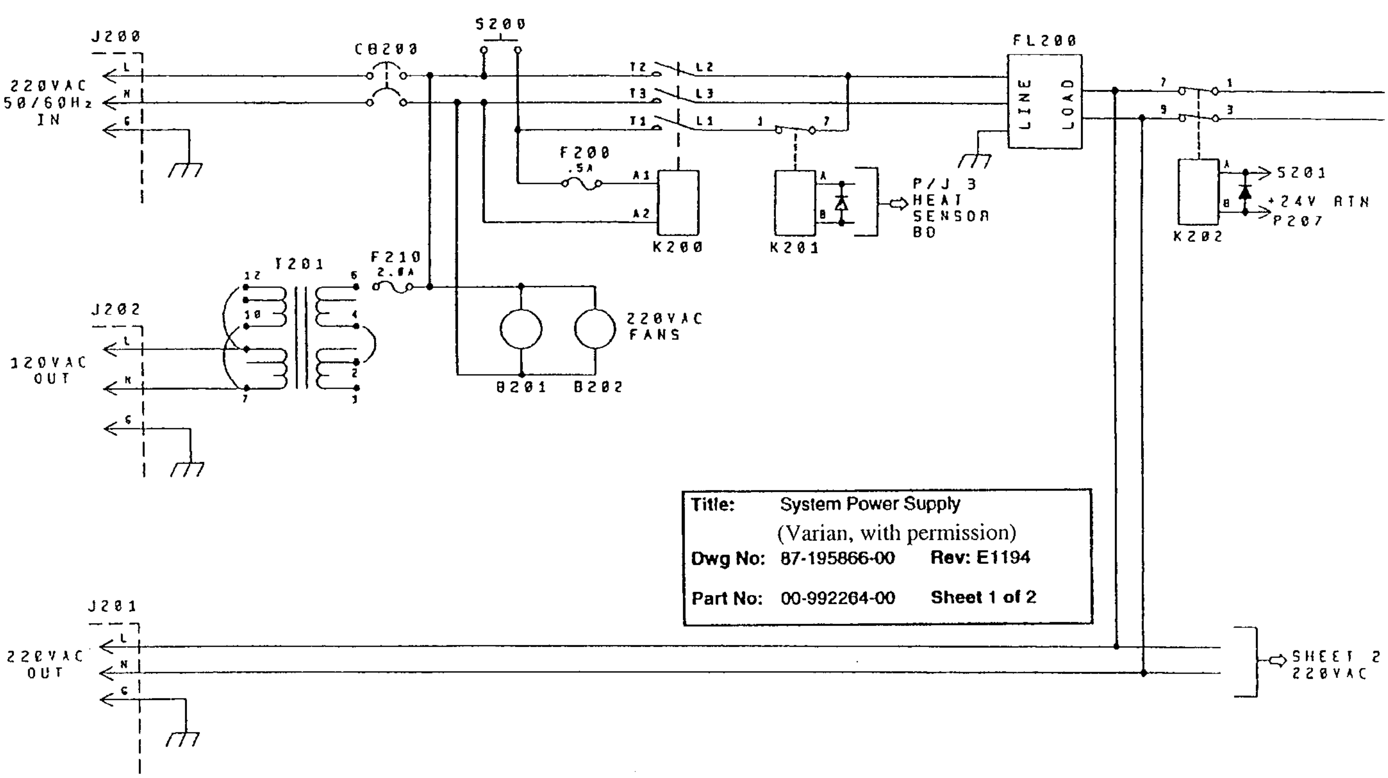

FIG. 2. Partial copy of the Varian schematics for the system power supply, showing the wiring of the K200 relay, the manual switch S200, the K201 relay which trips K200, and the J201 power plug which provides power downstream from K200. (Reproduction of the drawing with permission of Varian, Inc., Palo Alto, CA.)

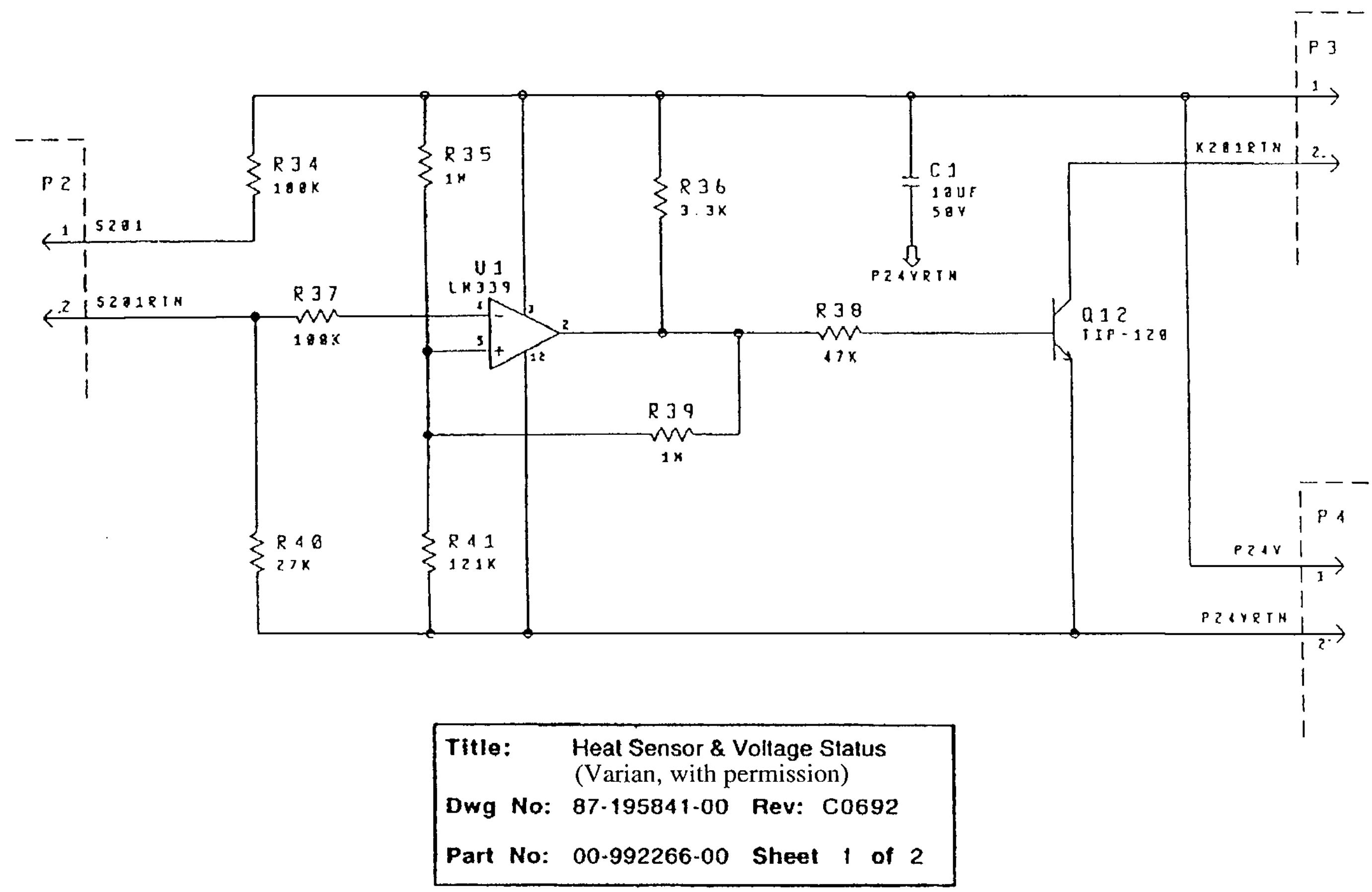

FIG. 3. Varian schematics of the heat sensor and voltage status PCB. (Reproduction of the drawing with permission of Varian, Inc., Palo Alto, CA.) The P2 connector provides the heat sensor input, P3 is the output to the K201 relay, and P4 supplies power.

The operation of the spectrometer involves external components, such as a nitrogen gas supply and variable temperature accessories. We power these from a spectrometer outlet which is itself powered via K200 (J201, Fig. 2). In particular, the nitrogen gas supply is controlled by an "open if powered" electro-valve; therefore tripping K200 shuts down the nitrogen gas supply. In contrast, we power the host computer independently of the NMR console, so that it is unaffected if K200 trips.

One situation where K200 trips is power supply overheating: the high temperature trips a relay, K201, which itself trips K200 (Fig. 2). The circuit which trips K201 is located on a printed circuit board (the heat sensor and voltage status PCB) which is conveniently located in front of the rightmost cabinet of the NMR system console (Fig. 3). We implement on this PCB a supplementary input for tripping K201, and this is the only hardware modification of the spectrometer.

In summary, tripping the K200 relay for whatever reason, including a power failure, shuts down the NMR console and all external equipment, including the nitrogen gas supply, without affecting the host computer. This leads to a reasonably fool-proof situation, which will persist until the relay is manually reset. In particular, the interruption of all power and of the nitrogen supply should avoid any drastic cooling or heating of the sample. Relay K201 provides convenient access for tripping K200. The shutdown function of the SPECMON monitoring system is the tripping of K201.

HARDWARE IMPLEMENTATION OF SHUTDOWN

In order to initiate shutdown, the macro `specmon` sets two output control lines, RTS and DTR, on the B serial (RS232) output of the host computer, which connects via a flat cable to a small box (about 3 × 7 × 10 cm) placed inside the NMR system console, from which a 30-cm long RJ45 cable goes to the heat sensor and voltage status PCB (Figs. 3 and 4). The box contains a simple electronic circuit for tripping K201.

The shutdown procedure is nearly independent of the NMR console. In particular, reliance on the RS232 port avoids any dependence on the NIC interface connection between the host computer and the built-in computer, or on the built-in computer itself. This reduces the chance of a catch-22 situation in which a failure of the NMR console would interfere with the execution of shutdown. However, the shutdown circuit does, like K201 itself, make use of a 24V power supply of the NMR console.

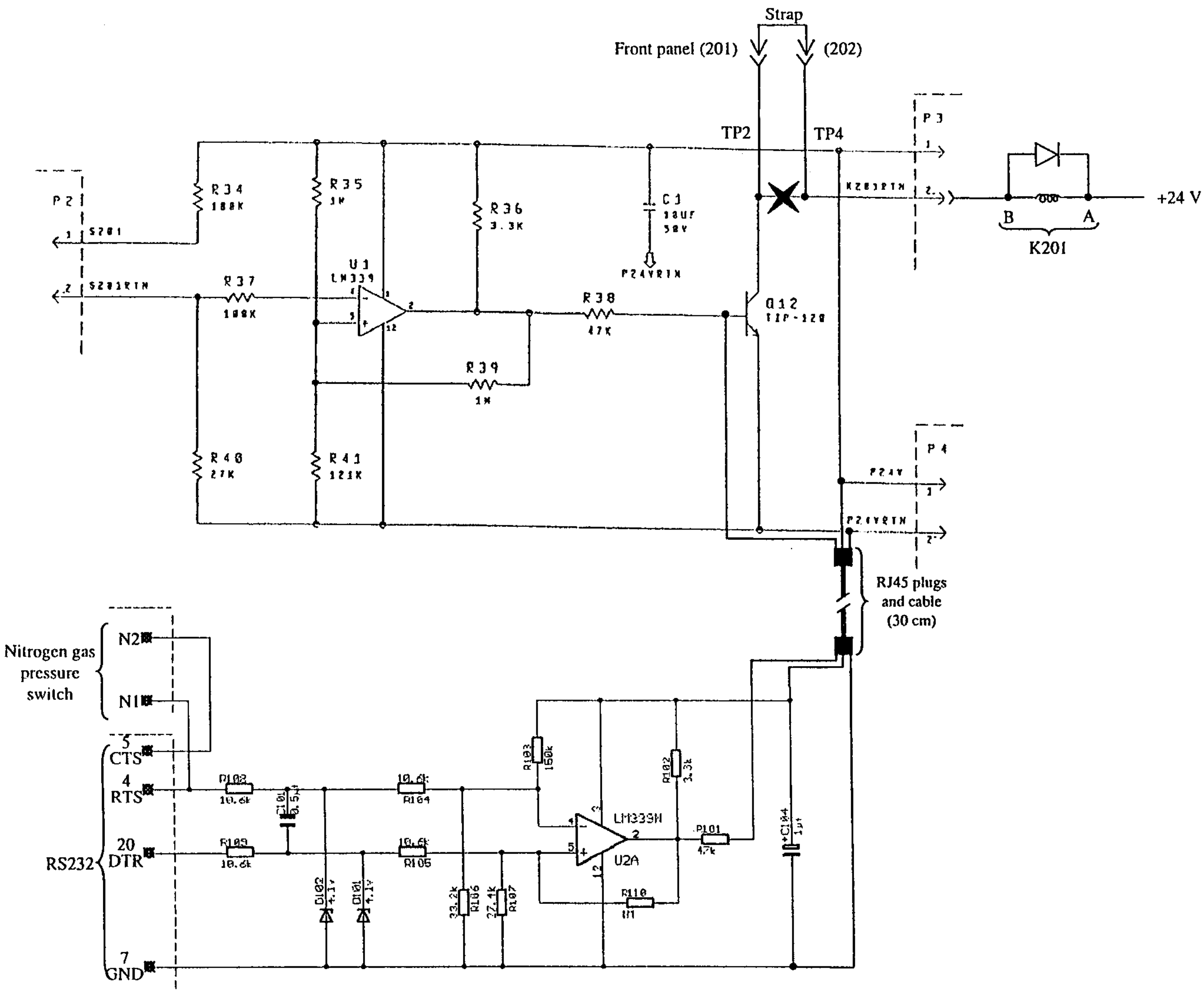

FIG. 4. Schematics of the modified heat sensor and voltage status PCB (reproduction of the drawing with permission of Varian, Inc., Palo Alto, CA) and of the supplementary electronics to which it is connected. Test points TP2 and TP4 have been disconnected from their original connections (to ground) and used for connecting the strap (normally a short; replaced by a 33-kΩ resistor for testing purposes) which is available on the front face of the NMR system console. An RJ45 plug provides power to the second electronic circuit, which in turn feeds an "OR" input to Q12. The second circuit receives input from the RTS and DTR lines of the selected RS232 port of the host computer and sends its output to Q12. Independent of this circuit, CTS provides the host computer with a signal from the nitrogen pressure switch.

The heat sensor and voltage status PCB includes LEDs for visual control of various power supplies, as well as test points for voltage measurement. The latter are easily accessible: one need only open the main door of the cabinet.

Our electronic circuit is inspired from that in the heat sensor and voltage status PCB and connects to it: it activates K201 by a logical OR connection to the original triggering pathway. The output track to K201 is common to the two circuits (Fig. 4).

Modifications of the Heat Sensor and Voltage Status PCB

The modifications to the PCB are quite limited. They include:

1. Cutting the printed track which feeds K201, and rerouting the two ends thus created to two test point plugs, TP2 and TP4, which are disconnected from their original test point connections for the return (ground) lines of two +5- and +15V supplies. (These test points are dispensable since the ground connection is available from other ground test points.) In normal conditions, a short-circuit strap, placed directly on the front panel, connects the TP2 and TP4 plugs, thus restoring the original K201 triggering function. The strap can be replaced by a strapping resistor, in which case the current is too small to trip K201: the voltage across the resistor is used for testing without tripping! The strap is accessible as soon as one opens the main front door of the cabinet.

2. Adding an RJ45 plug, for connection to the supplementary circuit. Three leads are used. Two provide power from the PCB's Gnd and 24V supply to the supplementary circuit board.

The third connects the output of the supplementary circuit board to the base of the output transistor on the PCB.

The Supplementary Circuit Board

This board is housed in a small aluminum box with two connectors, placed in the NMR console. It connects to the Varian heat sensor and voltage status PCB via a short (30 cm) RJ45 cable and to the RS232 port on the host computer via a flat 25-wire cable which may be quite long, e.g., 5 m (see below for one independent function of this cable). The circuit (Fig. 4) consists essentially of an LM339 operational amplifier (op amp) with the appropriate input and output network.

The inputs to the op amp are the two output control lines RTS (RS232 line 4) and DTR (RS232 line 20) of the host computer serial port. We use port B, since port A may be used by Varian for maintenance. The input connection also includes Ground (line 7). The input network serves three functions:

—The Zener diodes limit the op amp input voltages to a range of 0 to +5V, providing values which are roughly constant across the voltage ranges specified for the RS232 and RS423 standards, but with a voltage differential large enough for noise protection (Fig. 5). The capacity for handling the two standards is motivated by the implementation of one or the other in the Sun Ultra 1 computer (jumpers J2104 and J2105 on the main logic board).

—Capacitor C101 screens the op amp inputs from a transient voltage differential between the circuit inputs (RS232 control lines RTS and DTR), such as might occur when the host computer is turned on or off, or rebooted.

—Connection of op amp input 4 to the +24V line via R103 ensures that the voltage at input 4 is larger than at input 5 in any of the three logical states (0,0), (1,1), and (1,0) of the RS232 control lines RTS and DTR, where (x, y) corresponds to x on RTS and y on DTR. In the RS232 standard, logical states 1 and 0 of the control lines correspond to positive and negative voltage, respectively. These three states generate zero voltage at the output of the op amp. Thus, the op amp output goes high only for a nontransient (0,1) input.

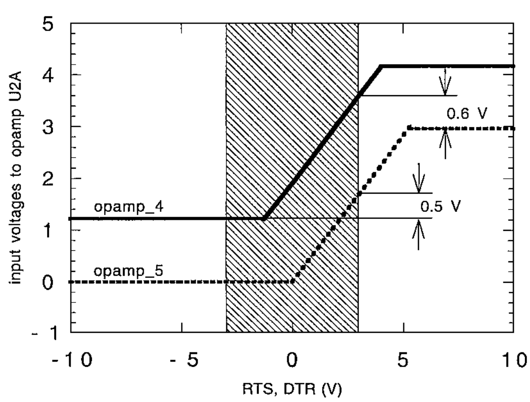

FIG. 5. Voltage at the inputs 4 and 5 of op amp U2A (Fig. 4) as a function of the voltage on the RS232 output lines RTS and DTR. In the range of allowed RS232 outputs, i.e., excluding the range (−3 to +3V), the logical settings (1,1), (1,0), and (0,0) drive the op amp output low, with at least a 0.6V margin on the inputs. A nontransient logical setting (0,1) drives the output high with at least a 0.5V input margin.

The output resistor R101 provides the OR logic which ensures that the original heat sensor function is maintained: transistor Q12 conducts (tripping K201) if the output of op amp U1 or of U2A is high.

Operation of the Shutdown Hardware

In normal conditions, no input other than (0,1) shuts down the spectrometer. Disconnection of the RJ45 cable, the RS232 cable, or both should not, and does not, trigger shutdown.

Rebooting, turning off, or turning on the host computer does not trigger a shutdown. Indeed, we measured the RS232 control lines RTS and DTR during these operations and observed that whereas the logical states of the lines may change, they are always identical, except for possible transients (which we did not observe). (However, see point 3 in the Bugs and Future Work section.)

The operation of the supplementary circuit board should be, as far as possible, insensitive to failures of the spectrometer. Although it fails if the 24V supply fails, the failure is gracious: it does not trip K201.

Nitrogen Gas Pressure Monitoring: An Independent Function for the RS232 Connection

The aim of the shutdown function is to provide an action in case of a critical situation, as monitored by the program set up within VNMR, on the basis of parameters supplied by VNMR. However, VNMR presently does not sense or respond to the nitrogen gas pressure.

We provide a signal to VNMR from a pressure switch set up in the nitrogen line. The switch is closed by nitrogen pressure. The leads from the switch go into the NMR console and connect to leads 4 (RTS, an output of the host computer) and 5 (CTS, an input to the host computer) of the RS232 port. It proves convenient to make the connection to the cable (via a two-connector plug) which links our shutdown circuit to the RS232 port of the host computer. Thus, CTS is connected to RTS if and only if pressurized nitrogen is present. The pressure signal CTS is handled by a SPECMON control routine, as explained in the Examples of the `specmon` Macro section below.

PROGRAM ARCHITECTURE: THE `SPECMON` MACRO

Installation of the software is described in the `install.eng` file. It consists in the setting of Solaris parameters related to the handling of the series ports, in some simple modifications of

VNMR macros, and in the creation of directories to which files are copied.

The VNMR macro, `/opt/specmon/maclib/specmon`, collects parameters, evaluates the situation, and decides, or not, to shut down the spectrometer. It runs continuously while VNMR is on. Nonexpert users have no option to turn it off, but they can run it in a stand-by mode. In this case, a reminder appears periodically on the host computer screen, to avoid the program remaining on stand-by by mistake or neglect.

Program Management

The specmon macro starts automatically when VNMR is started. It enters a loop which first waits for TIMER1, set presently at 60 s. It then checks the status, in the `/var/specmon/status` file. If the status is "on," the program runs normally and loops back. If the status is "off," it prints a message on the host computer screen (see page 297) and loops back. At the end of every loop, the `log1` file is cleared, and status, date, and time are written into it.

The procedure for starting the specmon macro is best examined directly on the macros. Special attention has been given to the effect of stopping or starting any number of versions of VNMR. The macro starts automatically with VNMR, as a UNIX background process. Prior to starting the macro, any remaining specmon process is killed.

Manipulation of the RS232 Lines

Shutdown is triggered when a control routine in the `specmon` macro sets the $panic variable to "on." If so, the submacro `rs232_sh` shells to the UNIX program, `rs232`, which can read–write the RS232 input–output control lines. It sets the output control lines to (0,1) and holds during TIMER2, presently 10 s. This will trip the K201 relay, so that the VNMR console and other systems shut down. It then calls rs232 again, resetting the control lines to (1,0). (One should note that a call to rs232 automatically sets the output lines to (1,1) before any further action.) Finally `specmon` resets $panic to "off." This procedure ensures that the spectrometer can restart once a failure has stopped it, and has been corrected!

Note. The `shell` command in VNMR macros always launches a Bourne shell (`sh`).

Timings

We wish to avoid any procedure which would rely on signals generated by the spectrometer. For timings, we shell to UNIX and make use of the "sleep" program. Note that timing is not dependable under UNIX.

Examples of the `specmon` Macro

For each parameter, the specmon macro includes a control routine, which places calls to its own submacros.

A minimum `specmon` macro, for testing purposes, would simply set or reset the $sm_status variable from the command line and then proceed to read it and act upon it.

A control routine for sample temperature would call a submacro which could for instance compare the sample temperature with the temperature posted in the current experiment.

Nitrogen pressure is a parameter which is not reported to the VNMR application software. As explained above, line 5 (CTS) of the RS232 port is a nitrogen pressure indicator. The control routine calls the submacro mon_nit. Using the `rs232` program, it sets the RTS and DTR lines to (1,0) and then reads line 5 (CTS). If and only if the switch is closed, the voltage on line 5 will be positive, as on line 4 (RTS), and it will therefore be read as logical 1. Otherwise CTS is disconnected and will be read as logical 0. Note that the (1,0) setting does not trigger shutdown.

PRESENT IMPLEMENTATION

We have set up the hardware as described. The design seems sound, inasmuch as there has been no incorrect triggering of shutdown, during months of normal operation, together with some cable disconnections, reboots, and strapping and unstrapping for tests.

BUGS AND FUTURE WORK

1. The present version of the `rs232` program requires the Sun serial port to be configured as RS232 rather than RS423.
2. For further protection from other users, one could inhibit access to the RS232 port by the appropriate EEPROM setting. Each call to the `rs232` program would lift the inhibition before operating and reset it after.
3. In a single port of a single Ultra machine, out of the 20 ports of 10 Sun computers tested, we observed that the Solaris default for the RS232 control lines RTS and DTR is set differently from the (1,1) value found on all other machines. This seems to be due to a hardware anomaly.
4. The specmon macro should run permanently, and therefore independently of which user account is running the spectrometer. On the other hand, the criteria for shutdown could in principle be user, sample, or experiment dependent: for instance, one experiment could require a specially strict supervision of the temperature; another might ignore the temperature setting entirely. The implementation of SPECMON should be compatible with these contrasting global–local aspects.
5. It is planned to post the SPECMON documents on the Web.

6. UNIX scripts could be used to make installation more automatic. In the Varian macros, shell calls could be replaced by a smaller number of calls to UNIX scripts.

ACKNOWLEDGMENTS

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