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APPLICATIONS NOTE NUMBER 2

The Nicolet 293 General Purpose Controller

Nicolet is pleased to announce its model 293 General Purpose Controller. The 293 is designed to take maximum advantage of the wired program features of the 1080 in controlling laboratory experiments. For instance, in pulsed nmr, even very small rf pulse widths do not vary appreciably because of memory cycle timing jitter.

The 293 Controller consists of four basic units: (a) programmer timer modules, provided at two per board; (b) a pair of 12-bit digital to analog converters on a board; (c) a digital input-output logic board; and (d) an eight input multiplexed 12-bit 200 usec analog to digital converter. A 293 consists of any number of any of these boards.

The heart of this system is the timer module, which can be loaded with any time in the range of 100 nanoseconds through 16 minutes under software control. Once each timer has a time specified for it, they can be configured so that each timer triggers the next and the last the first to provide a multiple pulse experiment. Thus, the software does not intervene in the pulse sequence until a pulse width or delay needs to be changed. At this point, the software can take over control, store the accumulated spectra in another part of memory or on disk, and modify the timer register.

For example, for the measurement of T_1 's by the Partially Relaxed¹⁻³ technique, the sample is irradiated with a 180° pulse followed by a delay time T , followed by a 90° pulse. The amount that the magnetization of each kind of nuclear species has relaxed since the 180° pulse is then measured by recording a free induction decay after the 90° pulse. From a collection of spectra taken at various T 's the relaxation time T_1 can be determined for each kind of carbon in a ^{13}C spectrum.

Using the 293, this experiment requires four timers providing times t_1 through t_4 where time t_1 is the width of the 180° pulse, time t_2 the delay time T , time t_3 the width of the 90° pulse and t_4 the length of time required for data acquisition and additional time to allow the nuclei to relax back to M_0 . This time t_4 is usually about 5 times the longest T_1 in the spectrum. Each of these timers triggers the next, and the end of t_3 also triggers the onset of data acquisition.

The 293 controller is set under software control with each of the four times t_1 through t_4 and data acquisition begins. After N sweeps are taken, the time t_2 is changed and a new set of spectra taken, and so forth.

The 293 controller is completely modular: each researcher can purchase only the boards he needs for his own work. The price is under \$2500 in most cases. Contact your local Nicolet sales representative for details.

Automatic Measure Modification

As discussed on page 13 of the FT-Nmr 1972 manual, the command GO will cause the 1080 to stop the stored program, go into the measure mode, take the number of sweeps on the Autostop counter, and return to software control. This makes it possible to control the entire experiment from the Teletype, and to Link the GO command into a list with the data processing commands. This feature is part of all digitizer plug-ins after serial number 52, but can be added to older plug-ins at nominal charge. The cost to U. S. customers is \$100 for a "do-it-yourself" kit, including instructions, or \$150 plus shipping for factory installation. Contact your local Nicolet sales representative or Nicolet in Madison for details.

PULSE1 - PULSE2 Under Software Control

It is possible for the 1080 to produce two pulses from the rear panel under software control with the addition of a PULSE1-PULSE2 modification board. With this board and appropriate software, the chemist can use these two outputs to trigger multiple pulse experiments, or to advance a digital plotter independently of the intensify pulse. This board comes as an add-on to the Teletype interface board and is connected to two of the unused BNC connectors at the rear of the 1080. It can be easily installed by the user, and is priced to U. S. customers at \$200. Contact Nicolet in Madison or your local Nicolet sales representative for details.

Summary of Data in Nmr Experiment

To print out a summary of the parameters used in an FT-Nmr experiment, to be attached to a plotted nmr spectrum, it is only necessary to punch out a tape containing the commands needed to complete the summary. To punch out this tape, turn the Teletype control to Local and turn on the punch. Then generate a length of leader by pressing the HERE IS key a few times. Then, type each command followed by a Return where necessary to close the constant entry routine and a Line Feed to separate the commands. This line feed is necessary because the FT-Nmr program clears the Teletype reader buffer each time before accepting a new command character.

For instance, to produce a summary tape which contains most useful information type the following series of commands, separated by a Return and/or a Line Feed as indicated by CR and LF.

```

SW (CR-LF)
TC (CR-LF)
T1 (CR-LF)
T2 (CR-LF)
SF (CR-LF)
OF (CR-LF)
MI (CR-LF)
PP (LF)
TP

```

At the end of this list, generate some trailer tape by depressing the HERE IS key a few more times. Then tear off the tape and label it the SUMMARY GENERATOR.

To use the Summary Generator tape, place it in the reader, with the first row of punched holes above the reader head. Turn the Teletype to LINE, start the FT-Nmr program if it is stopped, and turn the reader switch to START. A summary of the following type will be printed.

```

.SW* 5.000E3
SET DW= 100 X      1 USEC
EXACT SW= 5.000E3
.TC=-1.200E0

.T1= 30
.T2= 0
.SF= 2.514E1

.OF= -7.568E2

.MI= 0
.PP
  505 3.012E3 1.198E2 PPM 662
  523 2.968E3 1.180E2 PPM 940
  592 2.800E3 1.113E2 PPM 108
  625 2.719E3 1.081E2 PPM 748
  721 2.485E3 9.884E1 PPM 1000
 1524 5.249E2 2.087E1 PPM 856
 1611 3.125E2 1.242E1 PPM 845
 1739 0.000E-1 0.000E-1 PPM 142

.TP
A=-5.738E1
B=-1.415E2

```

Errata in the FT-Nmr Manual

Through a typographical malfeasance, the word "spectrum" was inadvertently perverted to "spectra" on pages 2 and 3 of the FT-Nmr 1972 manual. We apologize for this apparent, although unintentional, illiteracy.

Error in the T2 Trapezoidal Apodization Program (NIC-80/S-7202c)

It has been brought to our attention that the second apodization constant T2, which is supposed to force data points from address T2 to the last displayed address to zero misses the last two points. This error can easily be corrected by changing locations

	<u>from</u>	to
5045	3110461	3130461
5046	2451075	2471075

Errata in the Introduction to Programming Manual

The instructions listed under section d. on page 17 should be:

ACP	complement of the accumulator
MCP	complement of memory
ACM	accumulator plus complement of memory
CAM	complement of memory plus accumulator

The program on page 45 for displaying a section of memory under control of the pushbuttons should read as follows:

/SOFTWARE DISPLAY FROM PUSHBUTTONS

START,	STATUS	/READ STATUS WORD
	LASH 12	/SHIFT OVER READOUT STARTING BITS
	ANDA MASK	/MASK THEM OUT
	A+MA DSTART	/ADD ON 100000
	ACCM POINT	/STORE ADDRESS OF FIRST DATA POINT
	STATUS	
	LLSH 6	/SHIFT OVER SIZE BITS
	ACPA	/COMPLEMENT RESULT
	ANDAZ MASK	/MASK THEM OUT, IF 0, SET TO 16K
	ZERZ	
	MEMA K16K	/IF READOUT BITS = 0, DISPLAY 16K OF DATA
	ACCM COUNT	
DISPLA,	MONA	
	TACXD	/SET X-DISPLAY REGISTER TO -1
LOPP,	MEMA @ POINT	/GET EACH DATA POINT
	VDSH	/SHIFT FROM VERTICAL DISPLAY KNOB
	TACXD INCXD INTENS	
	MPOM POINT	/INCREMENT POINTER
	MMOMZ COUNT	/DECREMENT COUNTER
	JMP LOOP	/DO MORE
	JMP START	/DONE, REREAD SWITCHES
MASK,	36000	/MASKS OUT ALL BUT BITS 10-13
DSTART,	100000	/ADDRESS OF FIRST DATA MEMORY POINT
POINT,	0	/DATA POINTER
COUNT,	0	/NUMBER OF POINTS TO BE DISPLAYED
K16K,	40000	

Call for Contributions

Nicolet Applications Notes are published at pseudo-random intervals approximately once monthly. Nicolet users are invited to submit descriptions of new experimental techniques or 1080 programs for publication in these notes. Future notes will also contain some description of various laboratory set-ups utilizing the 1080. Send all such contributions to Nicolet in Madison, to the attention of J. W. Cooper.

Source Tapes

Some of the participants in the Nicolet User's Society have apparently been confused by the availability of source tapes of certain of the NUS programs. A source tape is a tape containing the ASCII characters comprising the Assembly language code. It is only interpretable by the Assembler program, and has no meaning whatever to the Binary Loader. Most programs do have source tapes available, but these are of no use to the user unless he plans to modify them from their current form. Tapes of spectra such as Snoopy, of course, have no source tapes, since they are not programs, but simply dumps of binary information from memory.

References

1. A. Allerhand *et al*, J. Am. Chem. Soc., 93, 544 (1971)
2. R. L. Vold *et al*, J. Chem. Phys., 48, 3831 (1968)
3. R. Freeman & H. D. W. Hill *ibid.*, 53, 4103 (1970)