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## A high-resolution multipurpose FT nmr spectrometer

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**Résumé.** — Un spectromètre de résonance nucléaire par transformée de Fourier est un instrument complexe, destiné à servir les besoins divers de nombreux utilisateurs. Avec au moins trois fréquences de résonance, des séquences d'impulsions variées et un traitement de données raffiné, l'instrument peut être un lourd fardeau pour l'architecte, le constructeur, et l'utilisateur. Nous nous sommes fixé pour but de réaliser un instrument dont l'utilisation ne nécessite qu'un minimum d'apprentissage, et dont l'entretien et les modifications éventuelles puissent être assurés aisément par d'autres que les constructeurs. Pour cela, nous avons fait appel systématiquement à l'utilisation répétitive de méthodes simples. En ce qui concerne la partie analogique du spectromètre, les trois voies — signal, référence, découplage — sont construites sur les mêmes principes : hétérodynage et utilisation exclusive de la fréquence intermédiaire pour les traitements du champ radiofréquence tels que génération d'impulsion ou changements de phase. La plupart des systèmes électroniques sont à bande passante large ; c'est notamment le cas des commutateurs émission/réception. Les commandes logiques sont transmises par un *bus*. Le spectromètre est multinucléaire. Il utilise la double détection, en phase et en quadrature. Le temps mort du récepteur est de 8  $\mu$ s, ce qui permet l'utilisation de l'appareil pour la résonance dans les solides. Le modèle choisi pour les sondes en simplifie la construction. L'interface entre la partie analogique et l'ordinateur utilise une structure de bus. Elle est facile à programmer et peut recevoir des fonctions supplémentaires. Les données sont enregistrées et accumulées sous la forme de mots de 32 bits, ce qui supprime toute saturation de la mémoire. L'acquisition des données est faite par programme. Cette méthode souple mais lente limite la largeur spectrale totale à 28,5 kHz. Les programmes sont écrits en FORTRAN. Ils font largement appel à des bibliothèques de sous-routines qui contrôlent les périphériques, et notamment l'interface du spectromètre ainsi que la console de contrôle. En conséquence les programmes se composent principalement d'appels (CALL) aux sous-routines, ce qui simplifie leur création, leur maintenance et leur lecture. Les communications entre l'utilisateur et les programmes sont rapides et détaillées. Elles ne font appel à aucune abbréviation. Une fois tapée la première lettre d'un mot de commande, celui-ci s'inscrit en entier sur la console. Les commandes disponibles sont présentées à la demande ; les programmes, enchâssés de façon fonctionnelle, fournissent d'abondantes informations de procédure. Aussi les manuels d'utilisation sont-ils superflus pour les opérations courantes. On notera qu'une console vidéo est indispensable pour établir ce mode de dialogue.

**Abstract.** — An FT nmr spectrometer is by definition complex : many users and uses, at least three nuclear frequencies, numerous excitation patterns and sophisticated data-processing methods. Hence such machines are often unwieldy for the designer, builder, operator and end-user. We have set ourselves the goal of building a machine which can be operated with hardly any training by users, and which can be easily maintained or modified by others than the building team. The design is based on the repetitious use of simple methods. In the analogic part, the three nuclear channels are built alike, pulsing, phase-switching etc. are all done at the intermediate frequency, and most systems are broad-band, notably the transmit/receive switches. A bus carries the logical controls. Receiver recovery time is 8  $\mu$ s, enabling solid-state type, broad lines to be measured. The spectrometer is multinuclear. Quadrature detection is used. A special design simplifies probe building. The interface between the analogic part and the computer is also built around a bus. It is easily programmed, and it can be extended. Data are accumulated as 32-bit words, thus avoiding memory saturation. The acquisition, under computer control, is easily programmed but limited to a total spectral width of 28.5 kHz. The programs, written in FORTRAN, make extensive use of subroutine libraries which manage the interactions of the computer and its peripherals, notably the spectrometer interface and the user's console. The programs are thus reduced mostly to CALL statements. They are easy to understand, maintain or create. User-software communications are fast, extensive, in English. Words are keyed-in by their first letter and printed in full. No mnemonics are used. Lists of available commands, program nesting and abundant information provided by the programs minimize the dependence on introductory manuals. Essential for the speed and ease of communications is the use of a CRT console, with graphics capability.

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Apart from such channel-specific features, the three channels are built in similar fashion. Any available nuclear frequency can be used in any channel. The nuclear frequencies originally provided are those of  $^1\text{H}$ ,  $^2\text{D}$ ,  $^{13}\text{C}$ ,  $^{31}\text{P}$ . Other nuclei can be included using a *Traficante scheme* [6].

The choice of the IF frequency results from a compromise. On one hand, a large IF frequency simplifies the rejection of the image frequency in the transmitters and receivers. On the other hand, a low IF frequency is an asset for the dynamic range of the receiver and its phase precision: the detection can be carried out by digital switches, and the IF can be amplified to higher voltages, thus reducing DC-offset problems of the detector and audio-frequency amplifiers. One solution [1] to these conflicting requirements is to use two successive IFs. In the present instrument a single *large* IF frequency is used, the detection being carried out *via* balanced mixers. The dynamic range is optimized by using as little IF gain as possible, i.e. just enough to overcome the noise of the low-noise, low-offset audio amplifiers.

In the nuclear frequency stages, broad-band components are used wherever possible. For instance the signal and decoupling power amplifiers are broad-band. So are the transmission/reception switches, this being achieved by the use of active PIN diodes (UNITRODE 6606B) which can easily switch powers in the kW range, thus obviating the need for narrow-band protection circuits or enabling cruder ones to be used (Fig. 2).

On the other hand the preamps are necessarily narrow-band, *per se* or by adjunction of filters.

For solid-state experiments it is important to achieve a fast recovery time of the receiver. In the

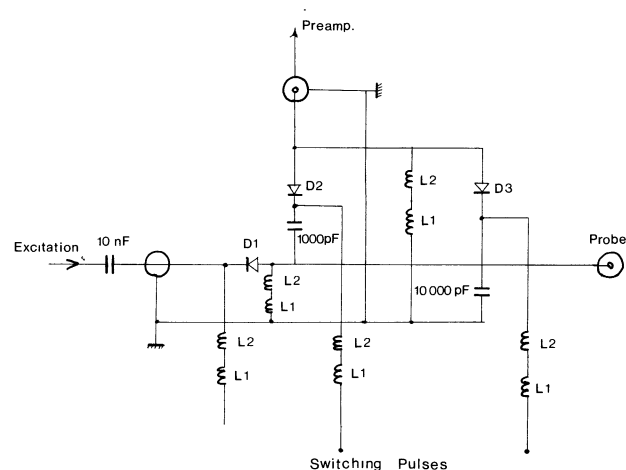


Fig. 2. — Broad-band PIN-diode transmit/receive switch.  $D_1$  and  $D_2$  are Unitrode UM6606B.  $D_3$  is Hewlett-Packard 5082-3039. For  $D_2$  two diodes in parallel are used.  $L_1$  is a 6  $\mu\text{H}$  inductance.  $L_2$  is 3 turns on a ferrite core (10 mm o.d.). The switching pulses turn  $D_1$  and  $D_3$  on and  $D_2$  off during the RF excitation pulse. This connects the probe to the transmitted ( $D_1$ ) while the preamp is isolated from the probe ( $D_2$ ) and connected to ground ( $D_3$ ) for protection. During reception,  $D_2$  is on,  $D_1$  and  $D_3$  are off.

signal receiver the transmit/receive PIN switch is followed by a series of balanced mixer switches in the IF stages, resulting in a dead time of only 8  $\mu\text{s}$ , for a pulse through-put of 1% of the receiver noise. This has enabled us, for instance, to carry out  $T_1$  measurements on broad lines, such as those of the protons [7] of TCNQ at 100 K or those of deuterons [8] in lamellar phases of fatty acids, without any modification of the spectrometer.

The various switches are actuated in a well defined time sequence which is adjusted to minimize switching transients. The possibility of such a scheme rests on two hardware choices. First the spectrometer has its own (rudimentary, non decoding) bus which provides for communication of logical states between the various analogic parts (pulsers, receivers, etc...). Second, we have designed a versatile pulser which not only provides a pulse of adjustable length but generates before and after this pulse a series of signals (called delays or more colloquially *shoulders*) of fixed duration, on different output lines. This is similar to the *pulse summer and extender* of Karlieck and Lowe [4]. A typical time diagram is shown in figure 3.

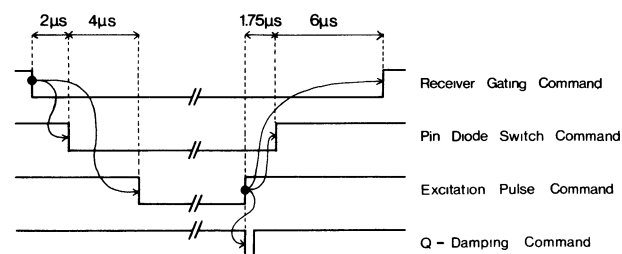


Fig. 3. — Time diagram of the pulse generator. The length of the excitation pulse is manually set. It is *shouldered* before and after at constant times with signals which are sent on the spectrometer bus for use by transmitter and receiver.

The lock channel receiver is nearly identical to the signal receiver. The lock is operated in the time-sharing mode, and the fast recovery of the receiver enables us to time-share at a high, constant, frequency (25 kHz). When in the homo-decoupling mode, the decoupling RF pulses are synchronized with the lock excitation.

2.2 THE PROBES. — For a multivalent instrument, it is unavoidable that many probes will be used. The probes are organized similarly to those provided by Bruker, but with the difference that in ours the probe-head which includes coil and circuitry may be disconnected from the cable assembly and temperature control unit (Fig. 4). This enables one to build probe-heads easily and cheaply, so that the coil design and size can be adapted to new experiments. Even visitors have built their own probe-heads, using the mechanical parts held in stock.

The electrical links between the two parts of the probe are by coaxial connectors which plug in

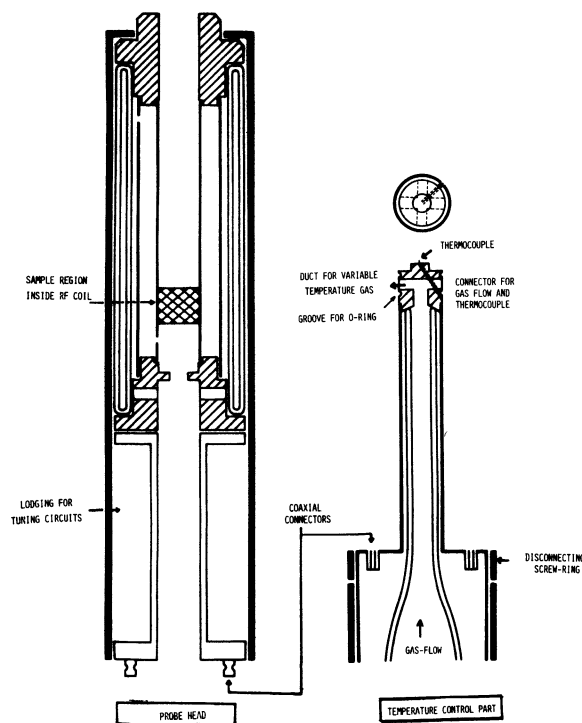


Fig. 4. — The probe assembly. The probe is in two parts. The temperature control and radiofrequency functions are well separated.

simultaneously. Three are for the signal, reference (lock) and decoupling channels, a fourth can be used for  $Q$ -quenching. The temperature sensor and heater are entirely contained in the temperature control part. The heating/cooling fluid flows from the temperature control part to the probe-head *via* a channel which is made gas-tight by O-rings.

The temperature control part of the probe is connected permanently to a mechanical arm along which are held: the connecting cables to the spectrometer, the thermocouple connector and a flexible stainless steel dewar transfer tube for the heating/cooling fluid. Cooling is by an exchanger coil immersed either in antifreeze fluid cooled by a finger refrigerator or in liquid nitrogen. The temperature controller is a Bruker.

When changing nuclei, one easily extracts the probe from the magnet bore with the mechanical arm. The probe head is replaced and the probe is reengaged in the magnet bore. It then slips up until its top abuts on the turbine assembly, thus always returning precisely to the same position. The entire operation lasts 30 s.

**3. The spectrometer interface.** — The spectrometer interface is based on an internal I/O bus which is linked to the I/O bus of the Data General Nova 800 computer through a general purpose I/O card (DGC 4040). The spectrometer is therefore considered by the computer as just another peripheral device and it is addressed by the standard DGC I/O instructions.

The interface is housed in a CAMAC crate and the various functions are implemented on CAMAC cards (see below for definition and discussion of CAMAC). Each card is separately addressable, using the addressing conventions of DGC software with suitable multiplexing. In this way supplementary functions are implemented easily, by the addition of a new card to which a new address is given.

The basic interface has two programmable timers and a two-channel, 12 bit A/D converting system including sample-and-hold amplifiers. These are used mainly for FID acquisition, but the A/D converter is multiplexed so that it can also be used for reading other analog signals, in particular the values of voltages controlled by a battery of potentiometers available to the operator and whose functions are program-controlled (e.g. for phase-correction).

The interface also has two D/A converters used notably to drive the X-Y recorder and various output registers by which logical signals are sent to the spectrometer, for defining RF phase, for lighting indicator lamps, etc.; input registers receive logical signals generated during FID acquisition, or corresponding to the position of manual switches.

As an example of supplementary functions, a fast timer with 256 32-bit words of memory, implemented on a CAMAC card, has been designed and added into the interface, as published [9]. It is used for generating complex pulse sequences.

The maintenance and repair of the interface are based on a series of test programs.

(It may be noted that Data General provides various I/O equipments and in particular interfaced A/D converters. These were however not fast enough for our purpose.)

We stated above that the interface is housed in a CAMAC *crate*. CAMAC is a complete interfacing standard, described in IEEE standards [10], and widely used in elementary particle physics instrumentation. When our instrument was designed, the equipments available in CAMAC standards were limited and the software procedures for addressing CAMAC were not well standardized nor widely implemented on minicomputers. Thus basing the interface entirely on CAMAC would have increased the development work, hence our decision to limit our involvement with CAMAC to the housing of the interface. The situation today would be different, as discussed in section 6.

#### 4. Data processing. — 4.1 GENERAL CONCEPTION.

— Basic to the design of the entire processing system is the choice of the method for data acquisition. We decided to manage the acquisition entirely *via* the minicomputer. That is, the memory would be that of the computer, and addition into memory would be carried out by the CPU. In other words, we chose not to build either a dedicated memory in the interface, or even a dedicated hardware adder accessing directly into computer memory. Our main motivation

was to minimize development work and time by keeping the interface functions to a minimum. Indeed the interface described in section 3 was built in less than 6 man-months. The programmed acquisition also has the advantage of being quite flexible. For instance it enables one to set up easily accumulation schemes (such as Cyclops) which involve successive additions and subtractions into memory. On the other hand the scheme suffers from a major drawback : the delays inherent in the programmed operations limit the acquisition rate, and hence, by the Nyquist criterion, the maximum spectral width. In the present system, the minimum sampling time is 35  $\mu$ s per ( $2 \times 12$  bits) complex word added into ( $2 \times 32$  bits), for a total spectral width of 28.5 kHz.

The following conceptual choices were also made :

— To simplify the programming of the accumulation by using memory words large enough (32 bits) to avoid any overflow, and therefore any testing and management of overflow.

— To use a high-level language (FORTRAN) for the application software, so that new programs could be implemented by non-specialized users.

— To use the operating system of the manufacturer without modification so as to minimize the programming effort.

Together with considerable emphasis on the efficiency, speed and ease of the user-program communications, these requirements and decisions determined the choice of the computer and its peripherals.

**4.2 CENTRAL PROCESSOR.** — The choice of the computer was based almost entirely on the speed of the tightest accumulating loop for  $2 \times 32$  bits. At the time, only the DGC Nova 800 and the PDP 11 could do the job in less than 40  $\mu$ s. The Nova was chosen because of price and delivery delay, and because the Operating System had a smaller resident core and was nevertheless more comprehensive. Another interesting feature of the NOVA is that the FORTRAN compiler provides an Assembler version of the programs, so that these can be optimized for speed if necessary.

**4.3 MEMORY SIZE AND ORGANIZATION.** — Using 32-bit words, an FID of for example 4 K complex words occupies 16 K words of 16 bits in memory. The corresponding spectrum occupies the same place. The programs for processing the data, plus the Data General operating system also occupy close to 16 K words. We chose to avoid the rather difficult and slow method of processing data on the disc. Rather a single memory layout was used for all operations, with the data in core at all times, enabling the data to be declared as a complex array common to all FORTRAN programs.

Clearly this method requires a lot of memory. For reasons of convenience and finance we chose the

maximum memory which does not require memory mapping, i.e. 32 K 16-bit words.

**4.4 PERIPHERAL DEVICES.** — To develop software efficiently, a disc-drive and a line printer are needed. A second disc-drive allows simple disc-to-disc transfer for back-up, filing and duplication of user's programs. Two Data General-supported DIABLO 2.5 Mbyte moving-head disc drives were installed.

We also acquired the hardware multiply and divide card for integers, and, in view of the Fourier transform, the same for floating point numbers (see below).

The application programs should ideally require no initiation. To this end they must provide clear information for possible actions (can I take a derivative ?), for detailed prompting (give the name of the nucleus) etc. A large flow of information between programs and user is then needed. The crucial step which makes the information flow possible is *the replacement of the slow teletype by a cathode-ray tube console*. The program writes out its part in full, and also gives guidance on request. The operator's commands are also displayed in full, although he types only as many letters (usually one) of each command as are necessary. The commands are presented in an easily recognized form. For instance : PRESENT PARAM., FREQUENCY OF FILTER, RATE OF RECURRENCE, START ACCUM., GRAPH, PHASE CORRECTION, MAKE CHART, ADJUST GAINS, etc.

The console is a Graphic Tektronix 4012, which is also used to prepare spectrum plots, including a frame with physical units (e.g. ppm) and a legend. These can then be transferred automatically to an X-Y recorder (Hewlett Packard 7041A).

Lastly, the user is provided with pilot lights as indicators of program status, whereas 12 switches and 4 potentiometers enable flexible inputs into program operations (see section on spectrometer interface).

**4.5 SUMMARY.** — The layout of the computer part of the spectrometer is shown in figure 5. The main characteristics from the application point of view are :

- user-program communications through the powerful and convenient medium of a graphic console ;
- programmed accumulation, with a loop time of 35  $\mu$ s for double 32-bit words. The spectral width is thereby limited to 28.5 kHz ;
- 32 K word memory. The maximum number of complex data points is 4 K ;
- mass memory in discs, used for both programs and data.

**5. The applications software.** — **5.1 CHARACTERISTICS OF USE.** — The software is first and foremost user-oriented. It uses extensively the dialogue possibilities offered by the cathode ray-tube console. As

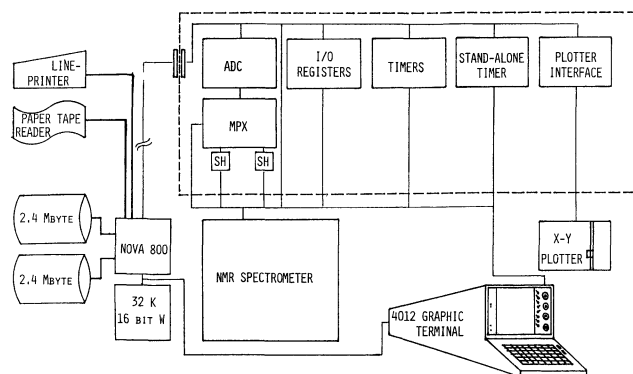


Fig. 5. — Configuration of the computer system. The interface is enclosed in the dotted line frame. On the display console are reticule controls, program-controlled LED lamps, and program-read switches and potentiometers. The interface is connected to the spectrometer through the simple, non-addressable spectrometer bus.

discussed above, the entire dialogue takes place in English and no abbreviations need be memorized. The software is organized as a series of modules. Each module has a list of commands available to the user (e.g. SPECTRAL WIDTH, CORRECT DATA...). The list is displayed on the console in response to keying-in of a question mark by the operator. Note that even this simple and obvious procedure would be intolerable with a teletype : it would use too much time and would soon spread paper over all available tables. The same reasons explain why the console easily provides information, e.g. « IN THIS PROGRAM, MINIMUM RECURRENCE TIME IS 4 MS », or « TMS IS 0 PPM, H<sub>2</sub>O 25C IS - 4.8 PPM. H<sub>2</sub>O SHIFTS 0.0125 PPM/C ». In this way the user is largely freed from the consultation of manuals. Knowledge of the commands in a broad sense is enough, for detailed instructions are obtained interactively from the computer at each step. Even a beginner is never stuck in a situation where he doesn't know what to do.

Great care has been taken to keep the dialogue in terms of *physical* parameters. Thus, if the user wants to take a proton spectrum in the hydroxyl region, he simply keys in the two limits of the spectrum in ppm, for instance - 7 and - 2. He next specifies the resolution or the time during which the FID is sampled. The number of sampling points is never mentioned. It is determined by the computer, using the Nyquist criterion. This number is not requested to be a power of two, and it is of no concern to the user. After the accumulation parameters have been set, the computer displays them, as well as others derived from them. A typical print-out is shown in figure 6.

The absolute ppm scale is computed (in triple precision integers) using as inputs the exact frequencies of the signal and reference (lock) transmitters, the chemical shift of the reference compound and the ratios of the  $\gamma$  values of the various nuclei which we have determined (Table I).

```

NUCLEUS: ..... H1
SPECTRAL WIDTH: ..... -7. 00E+00. .... -2. 00E+00 PPM
SAMPLES NUMBER: ..... 1380
ACQUISITION TIME: ..... 9. 99E-01 S
RATE OF RECURRENCE: ..... 3. 72E+00 S
TIME PER BLOCK: ..... 44 S
SPECTRAL RESOLUTION: ..... 1. 00E+00 HZ
SAMPLING INTERVAL: ..... 7. 24E+02 US
FID PER BLOCK: ..... 12
ACCUMULATED FID'S: ..... 0
SPECTRUM SAMPLES: ..... 4096
SUGGESTED FILTER: ..... 6. 90E+02 ..... 7. 70E+02 HZ (SINGLE & DOUBLE)
FREQUENCY OF FILTER: ..... 7. 00E+02 HZ (SINGLE)
BROADENING: ..... 0. 00E+00 HZ
PREVIOUS BROADENING: ..... 1. 00E+00 HZ
ORTHOG PARAM: ..... 0. 00E+00 ..... 1. 00E+00 (ORTH1&ORTH2)
DISP=ORTH2*(DISP+ORTH1*ABSP)
DATE (D/M/Y @H:M:S) ..... 17/9/79 @12:13:15
GENERIC NAME: Q348
COMMENTS:
POLY A CONCENTRATION=7 8E-2 M CO=0 T=348 K
ZEROED

```

Fig. 6. — A print-out of the parameters of an experiment, as they are presented on the scope after preparation of the experiment is completed. The operator-defined parameters are underlined. The true chemical shifts are keyed in, as well as the acquisition time, rate of recurrence and time per block. The program computes the number of sample points in the time domain. Note that this is distinct from the number of spectrum samples (frequency domain) and is not a power of two. The program also computes the sampling interval, the spectral resolution and the number of FIDs per block. Alternatively, any of these computed values could have been keyed in, instead of those chosen here which would then have been computed. The filter frequency is chosen among available values, following program suggestion.

Table I. — Relations between the magnetogyric ratios  $\gamma_H$ ,  $\gamma_D$ ,  $\gamma_P$ ,  $\gamma_C$  <sup>(a)</sup>.

$$\gamma_H/\gamma_D = 6.51439966 \quad (b)$$

$$\gamma_C/\gamma_D = 1.6380467 \quad (c)$$

$$\gamma_P/\gamma_H = 0.40480731 \quad (d)$$

<sup>(a)</sup> For all measurements the two nuclear frequencies are the excitation frequencies of the signal and reference (lock) channels, synthesized from the same crystal oscillator and determined simultaneously. For the first two determinations, the two compounds are part of the same solution.

<sup>(b)</sup> Measured as the ratio of H<sub>2</sub>O and D<sub>2</sub>O frequencies. The same result is obtained with C<sub>6</sub>H<sub>6</sub> and C<sub>6</sub>D<sub>6</sub>.

<sup>(c)</sup> Computed for the carbon and deuterium nuclei of TMS; based on the nmr frequencies of one aromatic carbon of ethylbenzene ( $\delta = -128.5$  ppm) and of the deuterons of acetone ( $\delta = -2.17$  ppm), whose measured ratio is 1.6382537.

<sup>(d)</sup> Computed for the phosphorus nucleus of 85% phosphoric acid and for TMS protons; based on the frequencies of water protons ( $\delta = -4.8$  ppm at room temperature) and of 85% PO<sub>4</sub>H<sub>3</sub> in a capillary, whose measured ratio is 0.40480520; corrected for bulk susceptibility [17], using volume susceptibility of  $-0.82 \times 10^{-6}$  for PO<sub>4</sub>H<sub>3</sub> and  $-0.72 \times 10^{-6}$  for water.

For processing the accumulated FID, different corrections are available, such as exponential multiplication, apodization and sine-cosine multiplication. These last operations sharpen (sine) or broaden (cosine) the NMR lines [11, 12].

One then proceeds to the fast Fourier transform (FFT). In what arithmetical format should it be carried out? The main difficulty is due to truncation errors, which can generate spurious images of large peaks. These should be kept smaller than the smallest peaks or, better, than the analogic noise. In practice



the choice is between floating point and double precision integer arithmetic. The latter suffers from serious scaling and truncation problems [13, 14a] and its widespread use is due mainly to the absence of a floating point peripheral in many nmr computers. On the other hand floating-point arithmetic largely avoids the problems mentioned [14b] and it has been chosen in the present instrument. With the DGC hardware floating point unit, the time for a floating point FFT of 4 K complex points is about 15 s. To achieve this speed, the FFT was first programmed in FORTRAN, and the Assembler version provided by the compiler was then *hand* optimized. The optimization reduces the running time by a factor of 5. The gain is mainly in the computation of the sines and cosines and in the bit reversal operation.

After the FFT, the spectra are automatically corrected for the response (amplitude and phase) of the audio amplifiers and filters and also for the delay between the end of the excitation pulse and the first sampling point (8  $\mu$ s as mentioned above). Thus, phase correction becomes a simple, one parameter operation.

Spectra are displayed on the console screen. The abscissa scale is in true ppm (i.e. the water peak falls at  $-4.8$  ppm), or in Hz if desired. Integration, zooming, etc. are provided.

Spectra are stored on disc along with the accumulation parameters. They are reproduced on paper using the programmed XY recorder.

**5.2 PROGRAM STRUCTURE.** — As mentioned earlier, memory is laid-out in a unique way, with specified places for data, application programs and Data General's Real time Disc Operating System. The application programs are called from disc as necessary, without perturbation of the data. The feature of program chaining enables one to introduce new programs easily. Overlays have been systematically avoided.

All the programs are written in FORTRAN. They are all based on a table of commands, and make use of large subroutine libraries.

The subroutines are optimized for speed, and are general enough for use in most of the programs. For instance, the table of commands makes an extensive use of strings of characters, the manipulation of which is quite difficult in FORTRAN IV (but not in the latest ANSI 77 version of FORTRAN). We therefore developed a string processor (written in Assembler), based on the representation of a string of characters by a descriptor (two 16 bit-words) which provides three pointers to a string buffer where the characters are kept [15].

The main programs and their chaining connections are shown in figure 7. The spectrum and FID display programs use our speed-optimized version of the Tektronix graphics library. Data storage uses the very convenient Data General disc filing system.

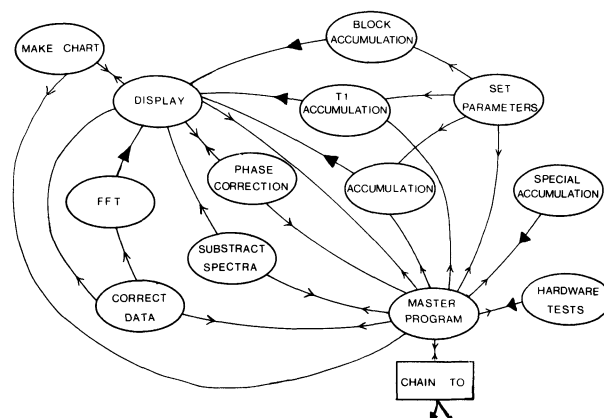


Fig. 7. — Linking of the various programs. The heavy arrows indicate an obligatory exit path. Besides the usual nmr programs, the user has easy access to hardware tests, to programs including special pulse sequences (SPECIAL ACCUM), or to any other program he may wish to write (via CHAIN TO). All the subroutines written for the nmr programs are available for such programs, which can therefore incorporate the convenient features of the nmr programs described in the text.

**6. Updating the design.** — The basic design of the instrument described above was frozen in 1973. In this final section we discuss briefly how we would change the design today.

We think there is nothing to change concerning our user-oriented philosophy. Each of our visitors has been delighted at the conveniences provided by the instrument, compared to what he is used to. The only changes one would provide are *more of the same*.

A magnet chosen among those available today would have better homogeneity and use less helium; hopefully it would hold its design specifications and be delivered within a reasonable delay.

No profound changes would be brought into the spectrometer. Frequency generation would make more use of single-side band techniques, with the help of wide-band phase shifters. Programmable audio filters would be used. (As they become available, multinuclear probes, better preamps etc. are incorporated in the present spectrometer.)

On the other hand, considerable changes would be brought today into the data processing equipment. This is due mainly to the possibility of building an elaborate interface with off-the-shelf CAMAC equipment, at a reasonable price. The interface would include a dedicated acquisition and accumulation module, with its own 24-bit word memory (available up to 64 K words), plus of course converters, multiplexers etc., all available in CAMAC. The main CAMAC module which must be custom-built is an Autonomous Function Controller (AFC) which would read the ADC and present its value to the adder included in the memory module. Such AFCs can be designed easily by using the large programmable read-only memories available today.

The accumulation would then be entirely auto-



nomous, and much faster than in the present design. The minicomputer would be involved only in the initialization and in the transfer of data onto disc, which would take place using standard FORTRAN CAMAC software [16]. The computer would be free for other tasks (such as processing earlier experiments) during the accumulation periods.

How would one choose the computer today? An important innovation is the existence of field-proven virtual memory management. This means that the maximum number of points of the FID and of the spectrum is nowadays set not by the amount of core memory but by the logical addressing space.

There is then a strong pressure to choose a computer with 16 bits (or even 32 bits) of logical address, in contrast to the 15 bits available in the Nova and PDP 11 lines.

A general-purpose mini, liberated from the chore of data acquisition and able to perform the FFT of the FID in a reasonable time is probably a powerful and underused machine. Now that good time-sharing software is provided by many manufacturers, it could also be used for other tasks in the laboratory. In turn, this may orient one's choice towards a more powerful system, in terms of peripherals, or of computer word length (16 *versus* 32 bits).

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