PRELIMINARY

1080 STORED PROGRAM OPERATIONS FOR FOURIER TRANSFORM NMR

The following is a preliminary list of the stored program data processing subroutines that can be called individually from the teletype by means of a two letter keyboard entry. All subroutines unless otherwise specified operate on the data displayed on the CRT and therefore the data indicated by the STARTING and SIZE MEMORY READOUT ALLOCATION pushbuttons.

Teletype Command

Operation

BC

BASELINE CORRECTION -- The DC level of the FID signal is restored to zero by means of a Simpson's rule integration routine to find the average value of the FID signal and then this value subtracted from all FID values. This results in an FID signal with equal positive and negative areas about a zero baseline. This subtoutine is automatically called and performed as the initial operation in the EXPONENTIAL MULTIPLICATION subroutine.

EM

EXPONENTIAL MULTIPLICATION -- The FID signal is multiplied by an exponential function on a point by point basis. The time constant of the exponential function may be positive or negative and of any arbitrary magnitude and is set into the subroutine by typing TC.

See description of TC command. Multiplication by a positive value time constant will improve the resolution of the Fourier transformed FID signal at the expense of signal-to-noise ratio and multiplication

by a negative time constant will improve the signal-to-noise ratio of the Fourier transformed FID signal at the expense of resolution.

TC

of an arbitrary value for the time constant in the EM operation. The time constant value should be determined by the amount of attenuation or amplification (negative or positive value) desired at the end value of the FID signal. For example, an entry of -2 will cause the FID signal to be multiplied by an exponential function whose value at the end address is e^{-2^n} (approximately 13% of its original value).

The entry can be made in fixed integer format having up to 5 digits and a decimal point between any digits. The entry is terminated by typing RETURN.

FT

FOURIER TRANSFORM -- The displayed FID signal is operated on by an in-place fast Fourier transform algorithm with the real and imaginary components of the result occupying the first and second half of the memory section in which the FID signal was displayed.

РC

PHASE CORRECTION -- Both the real and imaginary components of the transformed FID signal can be rotated along the complex plane to correct for phase distortions introduced by the spectrometer/data system. The rotation can be by means of a frequency dependent function with the zero and first order coefficients being entered by typing PA and PB.

PA

ZERO ORDER PHASE CORRECTION COEFFICIENT -- Typing PA causes the teletype to respond A= whereupon the operator enters the frequency independent term for the phase correction operation. This value is usually dependent upon the setting of the phase detector control of the spectrometer. This value is remembered for all PC operations until a new value is entered. The number entered is the number of degrees of rotation required to phase correct low frequency values. Format of entry is identical to that for TC.

PB

1ST ORDER PHASE CORRECTION COEFFICIENT -- Typing PB causes the teletype to respond B= whereupon the operator enters the first order frequency dependent term for the phase correction operation. This value is usually dependent upon the delay between onset of FID signal and the start of data accumulation and also on the characteristics of the input filters. This value is remembered for all PC operations until a new value is entered. The number entered is the difference between the number of degrees of rotation required to correct low and high frequency values. Format of entry is identical to that for TC.

MC

MAGNITUDE CALCULATION -- This subroutine computes the square root of the sum of the squares of the real and imaginary components of the Fourier transformed FID signal and replaces the imaginary component with the magnitude calculations.

DT

DATA TRANSFER -- This subroutine permits the transfer of stored data from one section of memory to another and to add or subtract portions of one section of memory to or from another section of memory. The 1030 main frame READOUT MEMORY ALLOCATION switches determine the Acceptor group of memory, i. e., the section of memory to which data are to be transferred and the MEASURE MEMORY ALLOCATION switches determine the Donor group of memory, i. e., the section of memory from which data are to be transferred. After typing DT the teletype responds DM= and the operator enters a multiplier which he wants the Donor data to be multiplied by.

LI

LINK -- This allows any of the above steps to be typed on the teletype and to be automatically executed in the order entered when AU is typed. The list of commands are terminated by typing two successive RETURNs on the teletype.

AU

AUTOMATIC -- Executes all commands entered under the LI operation in the order entered.

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INSTECK METTURY

INSTECK LIMIT

LL - LOWER UMIT

UL - UPPER LIMIT

AP

AN