① c:\> cd \ tbasic ↵
② tbasic ↵
③ old \ "esrplay.mds"

reg ↵
(1)
old

00

ESRPLAY

Abstract. The following stuff is something like manual for a new program for aquisition, storage and processing of ESR spectra.

General information

Name of the most advanced version available by the date:

ESRPLAY.001

Location: All IBM-compartible computers, root directory of disk C.

How to start the program :
1. If you need to use HP plotter, activate RS232.com program
2. Start TBASIC
3. Load the program using "OLD" command
4. Enter "RUN" to start the program.

How to quit : Press CTRL and C keys simultaneously.

How to restart the program without loss of information already stored in memory: RUN 23.

General principles

Commands. Each operation is performed after entering of one of the acceptable commands listed below in response on "ENTER COMMAND" request. **Only first three symbols are used to recognize a command.** The program comes in this regime after start, restart or completion of previous operation. To enter command type its name and press "ENTER", then obey program's requests.

Registers. Spectra can be loaded and processed in any of 10 absolutely equivalent registers numbered from 1 to 10. Maximum spectrum length is 3000 points. Any command excluding subtraction and least squares fitting procedures involves only one register named active register. Default active register number is 1. To change active register use "REG"command (see below).

Description of commands.

EXP*AND* Expands or compresses the spectrum on screen according to entered distance between Fremy peaks. Once executed, influences the spectra plotted from all registers. Doesn't change spectra in memory.

SHI*FT* Shifts the spectrum on screen horizontally according to entered new Fremy peak position. Nothing happens with spectra in memory.

HPP*LOT* The same as **PLOT** but using HP plotter as output device. SCALE , EXP and SHIFT commands are also valid. Don't forget to run RS232 program before loading TBASIC!

SAV*E* Writes spectrum from active register on disk. Works like the same facility of "ESRTAK" series of programs. Double integrals are also stored, if calculated. If not, the reserved variable retains zero value. **NOTE: files, written by this program, are not compartible with "ESRTAK" or "ESRADSUB" programs.**
compatible store — for ESRADSUB program

LOA*D* Loads disk files written by this program into active register.

OLD Loads disk files written by "ESRTAK" or "ESRADSUB" programs into active register.

SUB*TRACT* Adds or subtracts ESR spectra depending on the sign of weighting factor. No matter, were the spectra recorded at the same scan range or not. A register reserved for the result becomes active after the procedure is done. It is also automatically plotted on screen. **Note: one may use the same register for initial and calculated spectra, for example, to subtract background. However, remember, that initial spectrum will be lost after operation, when doing this.**

FIT Performs least squares fitting of an experimental spectrum using other spectra as basis functions. No matter, were spectra recorded at the same scan range or not. Basis functions must occupy the registers with sequential numbers without any lapse. Procedure also requires to define the area to be fitted by entering the coordinates of left and right boundary points. First Fremy peak is treated as the origin of coordinate system. Points from the left and right sides of this peak are associated with negative and positive numbers correspondingly. The register destined to store calculated spectrum becomes active after the completion of operation.

REG*ISTER* Displays the number of active register and allows to change it.

TAK*E* Used to record a spectrum from spectrometer into active register. Number of points to be taken must be specified in response on the program request. **At 4 min scan time full recorder chart length corresponds to 1200 points.**

BAS*ELINE* Performs baseline normalization of the spectrum in active register.

FIN*D* Uses statistical treatment to find boundary points of spectrum in active register. Looks for the first and the last statistically meaningful deviation of signal from its average value calculated on the wings of the spectrum. The point numbers found by this procedure are stored and used for integration. They are also shown on screen by vertical risks when spectrum is plotted. If this procedure is not used, first and last points of the whole spectrum are considered as boundary points.

REF*IND* Cancels the results of **FIND** command.

INT*EGRATE* Performs double integration of spectrum in active register. **The result is always displayed and stored in mV*G^2 units regardless of actual scan range.** Left and right first integrals are also calculated to check the quality of baseline normalization. Under ideal conditions they must be equal but practically it never happens. The 15% or less difference between two values may be considered as acceptable.

PLO*T* Plots the spectrum from active register using either default or preliminary specified screen settings. Default settings : position of the first Fremy peak 500, distanse between Fremy peaks 40 points, vertical scaling factor 1. Three following commands are used to change default settings.

SCA*LE* Enhances intensity of the spectrum on screen in the specified number of times. Spectra plotted from other registers will be subjected to the same transformation. Spectra in memory remain unchanged.