RAMOPN

Operating instruction for RAMOPN, a software package for the IBM PC compatible written by Doug Moffatt - National Research Council of Canada.

RAMOP is a program designed to perform a number of mathematical operations on digitized spectroscopic data. The data may be in one of several binary formats:

- a Bomem DA3 spectrum file.
- Digilab IMX spectrum file.
- Digilab FTS40/60 spectrum file.
- a native PC spectrum format (i.e. any output of the RAMOP program).

Also, there is a program XFORMAT that can translate data between the native PC format and any one of several common ASCII formats including a JCAMP-DX format.

Data filenames must have extension .dt and spectra that are to be processed as part of a series (Ntd > 1) must end in a decimal digit (no leading zeros). Do not enter the (.dt) extension when inputting filenames.

The user interface consists of a menu of numerical and text parameters
and a number of commands invoked through the function keys.

A numerical parameter is changed by highlighting it with the cursor (arrow keys) and entering the new value. Parameters may be zeroed with the space bar or incremented/decremented with the pageup/pagedown keys.
The **HOME** key positions the cursor at the first numerical parameter (Fnc).
The **END** key posistions the cursor at the first text parameter (in1).

The Fnc parameter controls the operation performed on the spectra as follows:

-1. - - - display in1
0.   no operation (except baseline correct if bs1 or bso is set)
1.   in1/In2
2.   sca * in1 * In2
3.   -log(in1/In2)   (base 10)
4.   sca * in1 + scb * In2
5.   10 ** (sca*in1)
6.   log(in1)   (base 10)
7.   Interpolate in1
8.   sca * in1 + con
9.   set in1 to con between st2 and en2
10. straight line interpolate between st2 and en2 in in1

11. trim spectrum to st2,en2
12. convolve in1 with first ncv points of in2
13. dump in1 to ou1 in text format
14. baseline correct using st2,en2 as baseline points (Con points are averaged around st2,en2 to calculate the baseline)
15. generate a running integral of in1
16. fourier shift in1 by alpha(= sca) of a datapoint
17. integrate between st2 and en2 and dump to ou1
18. interactive subtraction in1 + scb * In2. (st2-en2 are displayed stp-enp is subtracted and stored)
19. output width at con * peak height of highest band between st2, and en2
20. peak pick the top Npk positive (Lvl=1) or negative (Lvl=-1) peaks
23. interactive smoothing - functions 6 (trapezoid) and 9 (triangle^2)
24. interactive derivative - power = 3
25. interactive deconvolution - k= 1.5 to 3 by .25
27. undersample the spectrum; take every nth point (n=sca) starting at scb
28. automatic water vapour subtraction; In2 must contain a suitable spectrum for subtraction. This function uses the window St2,En2 for the calculation; 1730-1790 is often a good choice.
30. output Fourier transform of specified region
31. deconvolve with hw= sca, k= scb, lorentz fraction = con
32. derivative with pw= sca, brk= scb
33. smooth with brk= scb

Other parameters are:

  Stp,Enp - - starting and ending wavenumber (0,0 for full spectrum)
  Ntd   - - - - # of spectra to process
  Sca,Scb,Con - - variables used for certain functions
  Lvl - equiv. zero level (for functions that are undefined at zero -functions 1,3 or 6) i.e. values below lvl are set equal to lvl. Also set lvl to –1 to peakpick (fnc=20) negative-going peaks.
  Dl1,Dl2 - filename increments for in1 and in2
  Bs1,Bs2 - baseline correct (1), do not baseline correct (0) in1 or In2 before processing a value of (2) performs baseline correction using St2,En2 extrapolated to Stp,Enp.
  Bso - baseline correct (1), do not baseline correct (0) before output
  Ymn,Ymx - y values for fnc=-1. (0,0 to autoscale)
  Ils - lineshape function for fnc=31 or 33
  Ads - auto display flag, if ads = 1, spectrum is displayed after output
  Ftf - FT flag for function 31-33; 0= operate on spectrum 1= generate and output convolution coefficients
  Dla,Dlb,Dlc - change in sca,scb, con for each output file
  Ncv - # of convolute points for fnc=12
  in1,In2 - input files (in2 is needed for several functions).
  Ou1,Ou2,Ou3 - output files. Currently only ou1 is used.
  Pth - directory path for input and output files must be either NULL or a valid DOS pathname.

When all parameters have been set appropriately hit F1 to start processing. Other keys that are active in the menu are:

- F4 - display last output spectrum created
- F5 - quit ramop

- AF2 - pick in1 from a menu of data filenames
- CF2 - same as AF2 but scan directory first
- AF10 - jump to GPLOTC

When a spectrum is being displayed with the crosshair cursor, the following keys are active:
- cntl/x - input abscissa limits
- cntl/y - input ordinate limits
- F4 - shrink ordinate around cursor (or center mouse button)
- F5 - expand ordinate around cursor (or left mouse button)
- F6 - shrink abscissa around cursor (or center mouse button)
- F7 - expand abscissa around cursor (or left mouse button)
- F8 - return to initial display (or right mouse button)
- F9 - autoscale the display ordinate
- F10 - add another file to the display (maximum of 4)
- ALT/F2, CNTL/F2 - pick another filename as above
- PGUP/PGDOWN - change current file (if more than one is displayed)
- HOME - set st2 parameter
- END - set en2 parameter
- ESC - return to the menu

-Crosshair control defaults to the arrow keys unless a Msmouse driver is active and the DOS environment variable MOUSE=Y is set.

-This program uses a lot or RAM and probably will not function properly if TSR programs are installed that use a lot of system RAM. The current requirement is about 360 Kbytes of RAM. The program automatically senses the video hardware; about 60 Kbytes of RAM may be saved by putting EGA or VGA systems in Hercules mode before running the program.

- Current data size limit is 30000 points.

- Enter abscissa values in the order in which the spectra are stored. For most systems this will be low to high.

XFORMAT

Program XFORMAT

The purpose of this program is to permit translation of spectroscopic data stored in one of several possible ASCII and binary formats.

Possible input formats are:

0 - Binary i.e: Digilab IMX, Digilab FTS-40/60, Bomem DA3, or "NRC" binary.

1 - Single column ASCII; a single column of numbers the first three of which are the starting wavenumber, the ending wavenumber and the number of absorbance values in the file. The remainder of the file consists of absorbance values one per line (free format).

2 - Two column ASCII; a sequence of x/y pairs, one pair per line, consisting of the wavenumber and corresponding absorbance value.

4 - Four column ASCII; as in 2 except there are two x/y pairs per line. Abcissa values are still assumed to be equidistant and monotonic.

6 - Six column ASCII; as in 2 except there are three x/y pairs per line.

7 - Jcamp (X++(Y...Y)) format

Possible output formats are the same as possible input formats except that only one binary output format is supported - "NRC" binary - which is the one used by Ramop and Gplot (with Dat=1) and Jcamp is not supported.

GPLOTC

Operating instruction for GPLOT, a general purpose plotting package for the IBM PC compatible written by Doug Moffatt - National Research Council of Canada.

Menu variables have the following functions:

Xor,Yor - plot origin coordinates (inches).

Dat - type of data 0= xy data , 1= spectrum .

Xta,Yta - tic modulus values for x and y axes (set to -1 for auto).

Fnt - character font for plot (use 0=double or 1=single, 2=greek).

Plf - datapoint symbol +-12 (for dat = 0 only). A hundreds digit, if any, controls the symbol size; eg. for a large circle set plf=808.

Xsp,Xep,Ysp,Yep - limits for x and y axes. Setting both to 0 implies 'use the full limits of the data '.

Lht - size of characters (inches) for axes and annotation.

Xsl,Ysl - x and y scale lengths (inches).

Tkf - tick mark flag 0=in, 1=out, 2=both, 3=grid, 4=grid+tic.

Cur - display spectrum crosshair after plot (for spectra only).

Xxp,Yxp - scale xy data by 10^{xxp} (and/or yxp).

Lab - suppress(0) or enable(1) axes.

Pen - pen number (color number for color displays and pen plotters).

Lin - line type (0 to 6) for solid line plots (i.e. Plf=0).

Frm - suppress(0) or enable(1) frame around plot.

Aut - automatic plotting of temperature data at position xps,yps relative to spectrum origin. Aut=0 suppresses; Aut=1 plot every temp., Aut=2 every second, etc.

Ang - direction of text plotted with Annotate command. 0= horizontal, 1= vertical.

Ntd - number of successive spectra to plot.

Xnc,Ync - x and y offset per spectrum for stacked plots (ntd > 1).

Itf - interpolate flag; 1 = interpolate spectra before plot.

Bas - spectrum baseline correction flag. 1 = subtract linear baseline before display.

Fil - name of file to be plotted.

Ttl - string to be plotted along the top of the plot.

Pth - directory path to Fil.

Xlb,Ylb - labels for x and y axes. Special cases: (NULL) to suppress axis; Space to suppress axis label; CNTL/B to suppress axis label and tic label; Ending a label with the character "<" will move the axis to the other side of the plot.

Rot - plot direction 0=normal, 1= rotate 90 deg.

Spd - pen speed for hard copy (HP) plots (0-35).

Function key commands are :

F1 - - plot data in file Fil

ALT/F1 - escape to DOS temporarily. Type EXIT to return to GPLOT. This has limited utility because very little RAM is made available.

ALT/F2 - display possible input files and pick one.

CNTL/F2 - same as ALT/F2 but scan directory first.

F3 - annotate. Put Txt string at Xps,Yps

F4 - dump screen to Epson printer (screen dump only)

F5 (twice) - stop program

F6 - dump last screen plot to HP plotter or other destination specified by the environment variable HPGL.

F7 (twice) - clear current display

F8 - plot peak positions on last spectrum (50 peaks max)

ALT/F8 - more sensitive version of F8 (with shoulders)

ALT/F9 - remove the last plotted object

F9 - export plot to filename <Fil>.img

F10 - import (previously exported) plot from filename <Fil>.img the plot is appended to any current display

ALT/F10 - jump to RAMOP.

F2 - show and/or edit current display with crosshair in this mode the following keys are active:

m - mark this crosshair location.

v - join the last two marked locations with a vector. The type of vector is the current value of VAL (= 0 -5).

a - input and draw text at this location. Size is VAL/100.

A - same as 'a' with text plotted vertically. Size VAL/100.

b - draw the box defined by the last two marked locations.

e - erase all vectors having endpoints in the rectangle defined by the last two marked locations.

i - draw a vertical interval bar. The program will prompt for additional information.

k - plot point marker indicated by VAL (= +-13) ; see Plf.

o - set Xor, Yor parameters to this position.

f - linear regression on last x/y points plotted that fall inside the box delimited by the last two marked locations.

p - plot the last regression line (must follow f immediatly).

x or **X** - label this abcissa position. VAL controls char size.

cntl/z or **alt/z** - label last marked abcissa location with offset. VAL controls character size.

u - undo last operation that changed the display.

z - zap (hide) nearest object.

g - grab nearest object.

G - grab nearest object and hide it.

d - drop last grabbed object here.

h - redraw (unhide) all hidden objects.

r - redraw all visible objects.

R - rotate last grabbed object around crosshair VAL degre.

t - draw a down arrow here (size depends on VAL = 1-10).

T - draw an up arrow here (size depends on VAL = 1-10).

l - change last grabbed linetype to VAL.

L - change last grabbed color (pen #) to VAL.

s - Multiply entire plot around crosshair by VAL%.

S - Divide entire plot around crosshair by VAL%.

alt/o – (cntl/o) scale last grabbed object by VAL% (1./VAL%)

alt/x (cntl/x) - scale last grab. object x coord. by VAL% (1./VAL%)

alt/y (cntl/y) - scale last grab. object y coord. by VAL% (1./VAL%)

alt/t - translate (move) the entire plot the distance and direction defined by the last to mark (m) commands.

alt/g - display/remove a grid with spacing val/20 inches.

- **VAL** is changed by typing a 1,2,or 3 digit number.

- Objects are essentially any text string, vector, box, point marker or spectrum on the display.

- Labels and text may be **superscripted** by enclosing in '^' characters, **subscripted** by enclosing in underscores '_'. Enclosing text in bars '|' will cause it to be plotted using a **greek** font.
- **Pageup** and **Pagedown** keys are active in all menu fields. The function will be obvious.
- The **HOME** key positions the cursor at the first numerical parameter (Xor).
- The **END** key positions the cursor at the first text parameter (Fil).
- Crosshair control defaults to the arrow keys unless a Msmouse driver is active and the DOS environment variable MOUSE=Y is set. For keyboard the environment variable CSPEED (between 3 and 30) controls the behavior of the crosshair when the arrow key is pressed rapidly.
- Hard copy (F6) output defaults to a HP pen plotter on COM1, unless the DOS environment variable **HPGL=FILE**; in which case output goes to consecutive files - hpgl1,hpgl2 . . . etc. which contain HPGL graphics commands. These files may then be plotted on dot matrix printers or laser printers using commercial software packages written for that purpose or dumped to a HP plotter using the DOS copy or print command. Setting **HPGL=COM2** will redirect output to a plotter on COM2.

- Current data size limits are: for x/y data 2000 points and for spectroscopic data 4096 points. Datasets larger than 512 points are not interpolated (when Itf = 1).

- For technical reasons, spectra plotted with dashed lines (Lin != 0) may appear incomplete (or not appear at all) on the screen but will be plotted correctly with the hard copy command (F6).

Change a parameter by moving the cursor to highlight it (arrow keys) and entering the new value. Numerical parameters may be zeroed with the space bar.

GPLOT is a screen-interactive program the allows the user to create, edit and store figure-quality plots of data stored in one of several formats:
   1) Two column ASCII (Dat=0):
1) Two column ASCII (Dat=0):
- X/Y == a text file consisting of two columns of numbers (free format).
2) Spectrum (Dat = 1):
- a Bomem DA3 spectrum file.
- Digilab IMX spectrum file.
- Digilab FTS40/60 spectrum file.
- a native PC spectrum format (i.e. output of the RAMOP program).

PRINTGL

/F - OUTPUT FORMAT OPTION

/Fc[+ | - | * | i,j] - output format - default /FG

The F option specifies which output format to use. The format is chosen with a device character and a resolution modifier (-, +, *).
*, +, and - are allowed even where they have no affect. For bit maps you can choose a specific resolution in dots per inch. Resolutions here are given in horizontal x vertical dots/inch.
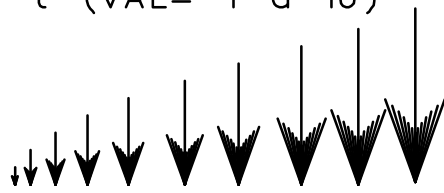
To return to DOS from a displayed plot, press Esc.

/F1	IBM Proprinter	120x72
/F1+	IBM Proprinter (2 pass)	120x144
/F2	IBM Quietwriter 2	240x240
/F3	IBM Quietwriter 3	240x240
/F4-	IBM LaserPrinter	150x150
/F4	IBM LaserPrinter	300x300
/F5	IBM Proprinter X24 printers	180x180
/F5+	IBM Proprinter X24 printers (2 pass)	360x180
/F6	IBM Proprinter X24	180x182
/F6+	IBM Proprinter X24 (2 pass)	360x182
/FB	bit map	100x100
/FBi,j	bit map	ixj
/FC	CGA display	62x25
/FE	128K EGA color display	62x45
/FH	Hercules graphics card display	70x45
/FL-	HP LaserJet printers	150x150
/FL	HP LaserJet printers	300x300
/FM	128K EGA B&W display	62x45
/FN	Epson 9 pin compatible printers	120x72
/FN+	Epson 9 pin printers (3 pass)	120x216
/FN*	Epson 9 pin printers (6 pass)	240x216
/FP	HP PaintJet	180x180
/FT	Epson 24 pin printers	180x180
/FT+	Epson 24 pin printers (2 pass)	360x180
/FT*	Epson 24 pin printers (4 pass)	360x360
/FV	VGA display	62x62
/FV+	enhanced VGA display 720x540 mode	70x70
/FV*	enhanced VGA display 800x600 mode	78x78
/FW	VGA display	62x62
/FW+	alternate VGA display 800x600 mode	78x78

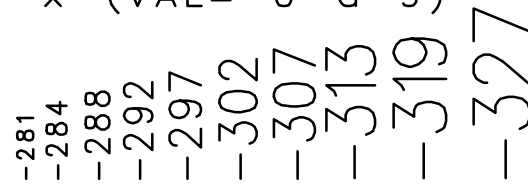COMPATIBILITY AND TECHNICAL INFORMATION

PrintGL will run on any IBM compatible MS-DOS computer. It will work in a region as small as 80K but may need more memory for high resolution or wide prints. 104K should suffice for the worst case black/white prints - 13.2 inches wide, 360x360 dpi. Color output requires an additional 32K or more for high resolution / wide prints. 184K is needed for the worst case. A larger region may make things go faster by allowing larger buffers and averting the use of a spill file.
By default PrintGL uses the BIOS printer interrupt to send data to a printer. If a file or device is specified for output then DOS 2.0
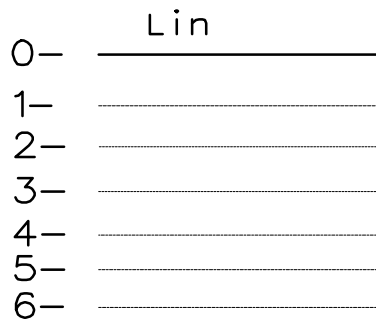
t (VAL= 1 a 10)

x (VAL= 0 a 9)

−281 −284 −288 −292 −297 −302 −307 −313 −319 −327

letras griegas

α β η δ ε φ γ χ ι

ϵ κ λ μ ν o π θ

ρ σ τ υ ϕ ω ξ ψ ζ

signos Plf

1— +
2— ×
3— ✳
4— ·
5— △
6— ▽
7— □
8— ○
9— ▲
10— ▼

11— ■
12— ●
13— ·
14—
15—

VAL vector

1— →
2— ⟸
3— ➤
4— ◄►
5— ◄ ►

Lin

0—
1—
2—
3—
4—
5—
6—

Pen #1	Pen #7	Pen #13
Pen #2	Pen #8	Pen #14
Pen #3	Pen #9	Pen #15
Pen #4	Pen #10	Pen #16
Pen #5	Pen #11	Pen #17
Pen #6	Pen #12	Pen #18

Pen #1	Pen #7	Pen #13
Pen #2	Pen #8	Pen #14
Pen #3	Pen #9	Pen #15
Pen #4	Pen #10	Pen #16
Pen #5	Pen #11	Pen #17
Pen #6	Pen #12	Pen #18