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Updated Users' Guide for RSAP – A Code for Display and Manipulation of Neutron Cross Section Data and SAMMY Fit Results

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Updated Users' Guide for RSAP – A Code for Display and Manipulation of Neutron Cross Section Data and SAMMY Fit Results. Version 6.

R. O. Sayer

1 Introduction

RSAP [1] is a computer code for display and manipulation of neutron cross section data and selected SAMMY output. SAMMY [2] is a multilevel R-matrix code for fitting neutron time-of-flight cross-section data using Bayes' method. This users' guide provides documentation for the recently updated RSAP code (version 6). The code has been ported to the Linux platform, and several new features have been added, including the capability to read cross section data from ASCII pointwise ENDF files as well as double-precision PLT output from SAMMY. A number of bugs have been found and corrected, and the input formats have been improved. Input items are parsed so that items may be separated by spaces or commas.

2 Overview

RSAP, which runs on the Linux and Digital Unix Alpha platforms, reads ORELA Data Files (ODF) and PLT files created by SAMMY. In addition, RSAP can read data and/or computed values from ASCII files with a format specified by the user. RSAP also can read cross section data from PENDF (pointwise ENDF) files generated by NJOY [3] or other nuclear processing codes. A peak search procedure and a procedure for performing a series of SAMMY calculations with different spin groups are built into the RSAP code. The code uses graphics routines from the PLPLOT [4] package.

Plot output may be displayed in an X window, sent to a postscript file (rsap.ps), or sent to a color postscript file (rsap.psc). Fourteen plot types are supported, allowing the user to display cross section data, transmission data, errors, theory, *Bayes* fits, and residuals in various combinations. In this document the designations *theory* and *Bayes* refer to the initial and final theoretical cross sections, respectively, as evaluated by SAMMY. Special plot types include Bayes/Data, Theory - Data, and Bayes - Data. Output from two SAMMY runs may be compared by plotting the ratios Theory2/Theory1 and Bayes2/Bayes1 or by plotting the differences (Theory2 - Theory1) and (Bayes2 - Bayes1). Two data files may be compared on a union energy grid by plotting the ratio Data2/Data1 or the difference (Data2 - Data1).

The term *plot* is used to denote a graphical representation of a combination of data, theory, errors, and Bayes from one data file. Several plots may be stacked in a single frame in a window (or page) with a common x-axis. RSAP also supports multiple frames in a window with each frame containing a separate plot. Up to 8 plots may be superposed, or overlaid, in one window with a separate normalization factor applied to each data set. The term *data set* denotes the numerical values of data, theory, etc. in one data file. Data may be plotted as histograms, points, small circles, or large circles. Theoretical values may be displayed as solid or dashed lines. Each axis may be linear or logarithmic.

Different colors may be specified for data, theory, Bayes, axes, and text. For example, the

specifier:

```
col y r g
```

sets colors for all plots to yellow for theory, red for Bayes, and green for data. These are the defaults. Note that white (**w**) shows well on the screen and in postscript plots, but white is invisible in color postscript plots. Different color combinations for different plots may be set with the `cst` specifer as illustrated by a detailed example in section 5.5.

Plots may be annotated in several ways:

- Values of resonance energies and widths read from a user-specified "PAR" file.
- User-specified X- and Y-axis label strings.
- User-specified annotation strings may be written at user-specified locations.
- A title string may be written above the plot.

Two text fonts, Simple and Roman, are supported. The default Simple font draws faster on the screen, and the Roman font is more readable for hard copy and publication quality plots. The size of axis labels may be scaled by the user.

RSAP produces an ASCII file **rsap.parcom** containing a formatted comparison of the user-specified PAR file with the file `SAMMY.PAR` and an ASCII file **rsap.ratexpth** in which energies, data, errors, theory, results of a SAMMY Bayes run, and percentage differences are listed. If `SAMMY.LPT` exists, the final value of the conventional CHISQ/N will be written on the plot.

RSAP reads input from either the keyboard or a file, and produces plots as specified by input quantities. To run RSAP on a DEC Alpha machine in the ORNL CAD farm, on **cpile**, or on **rsicclinux**:

```
rsap
```

or

```
rsap < inputfile
```

where `inputfile` is the name of your input file. On other systems you may have to create an alias or link such as `rsap ==> /home/ros/RSAP/v6/gorsap6` before running RSAP. Sample input files are listed and explained in section 5, Example Input Files. Plots corresponding to the example files are displayed in Figures 1-11.

The following sections include discussion of RSAP usage, plot types, specifiers, example input files, peak search and fitting, automatic spin group variation, and visual uncertainty analysis.

3 Use of RSAP

This section provides a brief introduction to some of the features of RSAP as well as descriptions of input data files and output plot file formats. More detail is given in Sections 4-8.

3.1 Getting Started

A good place to begin is `Example 1`, which plots data, errors, and the Bayes fit in one frame. Read the documentation in section 5.1 and run this simple case by typing "`exa 1,plot`" at the RSAP prompt. Then copy the input file to your directory, and try different options, types of plots, etc. Try one of your data files. Run example 2 to stack two frames in one window and example 3 to plot from two ODF files. All example cases may be run sequentially with the script:

`/home/ros/RSAP/EX/doexamples`

There are several ways to obtain "on-line" help. At the RSAP prompt type:

1. "`hlp`", "`help`", or "`man`" for a list of commands and help topics.
2. "`hlp cmd`" or "`man cmd`" for help with "`cmd`".
3. "`exa`" for a list of example files.
4. "`exa 6`" to list the contents of of example file 6.
5. "`exa 6, plot`" to run example file 6 and plot.
6. "`h`" for a list of specifiers and plot request types.
7. "`doc`" to open this users' guide in a separate window with Acrobat Reader.

3.2 Data Files

3.2.1 ODF and PLT Files

With release M6 of SAMMY, a SAMMY run automatically produces a double precision "PLT" file as well as the original single precision "ODF" file (ORELA Data File). These output files contain energies, uncertainties, experimental cross sections, *theory* , and *Bayes* values. Herein the designations *theory* and *Bayes* refer to the initial and final theoretical cross sections, respectively, as evaluated by SAMMY. RSAP can read both ODF and PLT files, but the user is encouraged to use PLT files wherever possible because all PLT files contain a header that specifies the units of energy values.

SAMMY now writes "new" ODF files that include a flag that specifies units of energy values. However, previous releases of SAMMY wrote ODF files with energies in units of eV (keV) if the maximum energy is less (greater) than 1 keV. These "old" ODF files did not include information on energy units. Thus, for "old" ODF files, the user must specify the energy units, either by the default (keV), or by selecting eV with the specifier "**ev 2**".

A maximum of 60000 data points is allowed in a given ODF or PLT file. Data points may be averaged before plotting by using the **avg** specifier.

All ODF files in the user's current directory may be opened by following the **odf** specifier with a space and asterisk e.g., "**odf** $*$". Similarly, all PLT files may be opened with "**plt** $*$".

3.2.2 DAT Files

RSAP can read data and/or computed values from an ASCII "DAT" file with a user-specified format; for example:

```
dat myfile.dat
```

Five quantities are read per record: x, y1, err1, y2, and y3. These quantities can be any set of numerical data; however, in order to use the same RSAP commands as those used for ODF and PLT files, the code makes the correspondences x ⇔ energy, y1 ⇔ data, err1 ⇔ error, y2 ⇔ theory, and y3 ⇔ Bayes. Note that the initial and final theoretical cross sections evaluated by SAMMY are denoted by the terms *theory* and *Bayes* , respectively. Thus the RSAP plot request "**1 dt**" will plot y1 (data) and y2 (theory) vs. x (energy). The default format is **(5e11)**, corresponding to the **csisrs** data format. Other formats are selected with the **fmt** specifier; for example **fmt (5e20.6)**. The user may specify axes labels pertaining to the actual information in the DAT file; for example

```
xlb time
ylb pressure
```

A maximum of 60000 data records is allowed. Data points may be averaged before plotting by using the **avg** specifier.

3.2.3 NDF Files

RSAP can read pointwise cross section values from an "NDF" file, an ASCII pointwise ENDF file generated by NJOY or other nuclear processing codes. For example, to read elastic (MT=2) and capture (MT=102) cross sections from a PENDF file named **mypendftape**

```
ndf 2, mypendftape
ndf 102, mypendftape
```

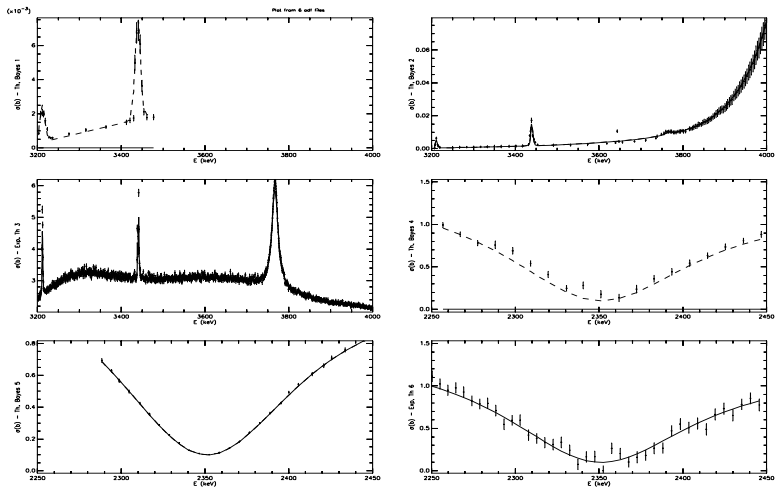
Appropriate axis labels may be specified; for example

```
ylb capture cross section (b)
```

A maximum of 60000 data records is allowed.

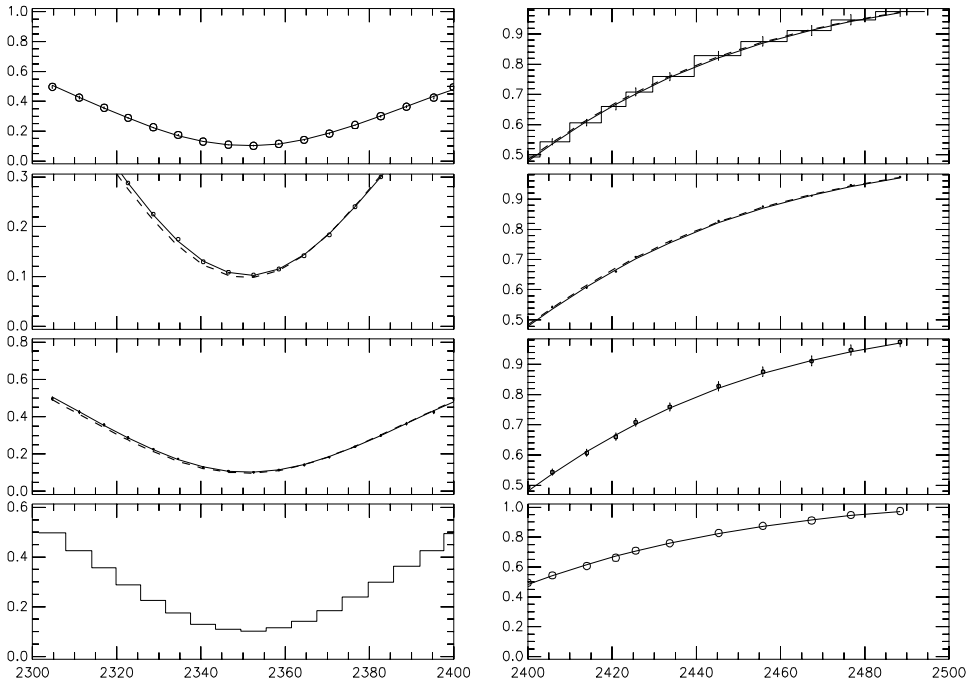
3.3 Multiple Plots in a Window

Multiple plots in a window may be accomplished by specifying more than 1 frame in either the x- or the y-direction through the "**nxy**" command. Each frame will contain a plot with unique x- and y-axes. For example, use "**nxy 2,3**" to plot 6 data sets in a 2 x 3 matrix in x and y.



Two to eight plots may be "stacked" in the same frame using a common x-axis. A given plot may include any combination of data, theory, and Bayes values. Examples 2 and 3 illustrate the use of the "**nxy 1,1,2**" command to stack 2 plots in one frame (see Figures 2 and 3). To plot 8 data sets, stacking 4 plots per frame in a 2 x 1 matrix in x and y:

nxy 2,1,4



3.4 Use of the oxp, oxs, and pan Specifiers

Before a plot can be sent to the user's screen, the output device and data file must be specified. Normally RSAP expects to read a device specifier followed by one or more "plot request" records. Thus, to plot data, errors, and bayes from data file 1 for 200 keV $< E <$ 300 keV, the input would look like:

```
x
1 deb 200.,300.
```

Alternately, the `oxp` specifier may be used to plot from one data file:

```
oxp 1 deb 200.,300.
```

To plot from data files 1, 2, and 3, for example, three plot request records must be input:

```
nxy 1,3
x
1 deb 200.,300.
2 deb 200.,300.
3 deb 200.,300.
```

This sends the frame of three plots to an X-window on the user's screen. Of course, at least three data files must have been read prior to the `x` command.

In each of the above examples, RSAP sends plot output to one X-window on the screen and waits for a "carriage return" from the user.

The specifier `oxs` allows the user to view two or more plots in separate X-windows on the screen. Thus, to plot from data file 1 in 2 X-windows with 200 keV $< E <$ 300 keV and 300 keV $< E <$ 400 keV, the input would be:

```
oxs 1 deb 200.,300.
oxs 1 deb 300.,400.
```

After an `oxs` specifier is read, RSAP sends the plot to the screen and processes the next input record. The `oxs` window remains on the screen until a "carriage return" is typed by the user.

The `pan` specifier may be used to "pan" through a data set by incrementing the x-axis limits by a specified amount. The arguments of `pan` are the initial minimum energy, width, and final maximum energy. To plot from data file 1 from 200 keV to 800 keV in steps of 100 keV:

```
pan 200.,50.,800.
```

RSAP will send 6 plots to the screen (200-300 keV, 300-400 keV, ...) in sequence, waiting for a user "carriage return" before sending the second and subsequent plots. If the maximum energy is omitted, `pan` continues to the maximum energy in the data set.

By default, data, theory, and bayes (dtb) are plotted from data file 1. To plot data, errors, and theory from data file 4:

```
pan 200.,50.,800.,4 det
```

3.5 Overlay of 2 or more Plots

RSAP allows up to 8 plots to be overlaid in the same frame using common x- and y-axes. A particular plot may include any combination of data, theory, and Bayes values. A normalization factor may be applied to each data set via the "**nrm**" specifier as defined in section 4. This overlay feature is most useful for showing general features of fits to several data sets. Example 9 illustrates the use of normalization factors in an overlay.

3.6 Preview in Encapsulated Postscript Files

With the PLPLOT package, the postscript files produced by RSAP do not contain a preview graphic. Thus, when these files are inserted into Word or Powerpoint documents, they do not display on the screen although they will print to a postscript printer. To obtain a screen display, an RSAP postscript file must be converted to an encapsulated postscript file (EPS) with a preview. This can be done on Unix or Linux with the utility **epstool**, on a Windows machine with **gsview**, or on a Macintosh with **EPS Factory**.

For example, on **cpile** the commands

```
epstool -t6p rsap.psc myplotp.eps
epstool -t6u rsap.psc myplotu.eps
```

will create EPS files myplotp.eps with a compressed TIFF 6 preview and myplotu.eps with an uncompressed TIFF 6 preview, respectively.

3.7 Plot File Formats

The color (monochrome) postscript file **rsap.psc** (**rsap.ps**) produced by RSAP may be converted to GIF, JPEG, or TIFF format with the **xv** program. For example, the command

```
xv -rot 90 -cmap rsap.psc
```

displays both **rsap.psc** and the xv control window. Click on "SAVE" in the control window and choose the file format in the SAVE window.

RSAP also produces a PLPLOT metafile, **rsap.meta**, that may be rendered with the **plrender** procedure described in Appendix D. For example, to make a color postscript file, **rsap_port**, in portrait orientation:

```
plrender dev psc o rsap_port ori 3 rsap.meta
```

For a white background:

```
plrender -dev psc -bg FFFFFF -o rsap_port -ori 3 rsap.meta
```

JPEG output (for PLPLOT version 5.1.0 and later) may be produced:

```
plrender -dev jpg -bg FFFFFF -o rsap.jpg rsap.meta
```

3.8 Union Energy Grid

Two data files with the same energy grid may be compared by plotting the ratio of cross section values Data2/Data1 or the difference (Data2 - Data1). The corresponding plot types are `12dod` and `12dmd`. If the two files have different energy grids, a union energy grid may be created:

```
uni icode, eulo, euhi
```

where `icode`= (2, 3, 4, 5) for (linear-linear, log-linear, linear-log, log-log) interpolation and the energy limits are `eulo` and `euhi`. The union energy values and the interpolated cross section and uncertainty values are written to files `rsap.union_dat1` and `rsap.union_dat2` using the format (2e20.10, e20.6). These files may be read and compared using the specifiers "`fmt (5e20.10)`", "`dat rsap.union_dat1`", and "`dat rsap.union_dat2`". Type "`exa 20`" at the RSAP prompt for a detailed example.

3.9 Greek letters, subscripts, and superscripts in axis labels

Axis labels may contain Greek letters, subscripts, and superscripts. Two example specifiers and the corresponding axis labels are shown below.

Specifier	Axis Label
`xlb x = #gG#u0#d/<#gG#u0#d>`	$x = \Gamma^0 / < \Gamma^0 >$
`ylb 39 * 2 #gp#u-0.5#d e#u-x`	$39 * 2\pi^{-0.5} e^{-x}$

The applicable control sequences are:

```
#u - move up to superscript (end with #d)
#d - move down to subscript (end with #u)
#gx - Greek letter corresponding to roman letter x
#fn - switch to normal font
#fr - switch to Roman font
```

The following table from Ref. [4] shows the mapping of the Roman letters following `#g` into Greek characters.

Roman	A	B	G	D	E	Z	Y	H	I	K	L	M
Greek	A	B	Γ	Δ	E	Z	H	Θ	I	K	Λ	M
Roman	N	C	O	P	R	S	T	U	F	X	Q	W
Greek	N	Ξ	O	Π	P	Σ	T	Υ	Φ	X	Ψ	Ω
Roman	a	b	g	d	e	z	y	h	i	k	l	m
Greek	α	β	γ	δ	ϵ	ζ	η	θ	ι	κ	λ	μ
Roman	n	c	o	p	r	s	t	u	f	x	q	w
Greek	ν	ξ	o	π	ρ	σ	τ	υ	ϕ	χ	ψ	ω

4 RSAP Specifiers and Plot Requests

RSAP input consists of "specifier" cards and "plot request" cards. At least one **plt**, **odf**, **dat**, or **ndf** specifier is required to define an input file. Other specifiers such as **nxy** or **npt** may be included to set various input parameters. A device specifier (**x**, **ps**, or **psc**) is required to set the output device. Note that the device specifier "**x**" sends the plot to an X plot window, the color postscript file **rsap.psc**, the monochrome postscript file **rsap.ps,** and the PLPLOT metafile **rsap.meta**. Specifiers **ps** and **psc** send output to postscript files only.

After a device specifier, RSAP expects one or more plot request cards. Plot request input consists of the data file number, plot type, emin, emax, ymin, ymax in (a2, a4, 4f) format. X- and Y-axis limits are denoted by (emin, emax) and (ymin, ymax), respectively. Axes limits default to the data limits. RSAP plot types and specifiers are listed in Tables 1 and 2, respectively.

Table 1: **RSAP Plot Types**

TYPE	**DESCRIPTION**
1 d	CROSS SECTION Data from data file 1
2 d	CROSS SECTION Data from data file 2
1 de	Data, Errors
1 dt	Data, Theory (INITIAL theoretical cross section)
1 db	Data, Bayes (FINAL theoretical cross section)
1 det	Data, Errors, Theory
1 deb	Data, Errors, Bayes
1 rt	Residuals, Theory
1 rb	Residuals, Bayes
1 bod	Bayes/Data
1 tod	Theory/Data
1 bot	Bayes/Theory
1 dtb	Data, Theory, Bayes
1 etb	Data, Errors, Theory, Bayes
1 tmd	Theory - Data
1 bmd	Bayes - Data
a d	TRANSMISSION Data from ODF file 1
b d	TRANSMISSION Data from ODF file 2
a de	TRANSMISSION Data, Errors
a dt	Data, Theory
...	...
12dod	(Data from file 2) / (Data from file 1)
12tot	(Theory from file 2) / (Theory from file 1)
12bob	(Bayes from file 2) / (Bayes from file 1)
12dmd	Data2 - Data1
12tmt	Theory2 - Theory1
12bmb	Bayes2 - Bayes1

Table 2: **RSAP Specifiers and Arguments**

SPECIFIER	ARGUMENTS	FORMAT	DESCRIPTION example
ann	kpl, ka, kacol, ann_string	i1, i1, i2, a40	Plot # for this string 1,2,3 for left, center, right above frame top 4,5,6 for left, center, right below frame top color annotation string `ann 14  This is an annotation`
avg	kaverage	i	# of data points to average before plotting `avg 12`
bug	kdebug	i	> 0 says print debug information
cap	capt_string	a64	Caption string : ≤ 64 characters `cap This is a caption`
cmf	cmf_name	a72	Command file name : ≤ 72 characters
col	kt,kb,kd,ka,kt	5a2	colors for theory,Bayes,data,axes,axestext one of “y”,“r”,“g”,“c”,“b”,“m”,“w” `col y r b`

cst	ctype,col(1-8)	9a	set theory,bayes,data colors for data file i
			`cst data, green, blue`
			`cst bayes, red, yellow`

dat	dat_name	a72	DAT file name : ≤ 72 characters `dat /home/xyz/u235/mydata`
doc			opens this document in a separate X-window
dsh	kdash(1-8)	8i	data dash patterns for data file i `dsh 1, 0`
ev	kplev	i	= 2 says data energies are in eV > 0 says resonance energies, widths in eV `ev 2`
exa	kex,(plot)	i,a	type script for example kex `exa 4` : type example 4 script `exa 4,plot` : run ex. 4 and plot
fis	kfis	i	= 0 says set fission widths to 0 for peak search `fis 0`
fmt	fmt_string	a72	format string for DAT files `fmt (5e20.4)`
fnt	kfont, fontscale	i, f	1 (2) says SIMPLE (ROMAN) font; axis labels scaled by fontscale `fnt 2`
hlp, help, man hlp	cmd		lists commands for which help is available prints “help” message for “cmd” `hlp plt`
lab	kodf, kdate, kchi	3i	= 0 : don’t write odf name, date, chisq/n `lab 0 0 0`
log	kx, ky	2i	kx (ky) > 0 says logarithmic x (y) axis `log 0 1`
lpr			sends rsap.ps to default printer

Table 2. RSAP Specifiers and Arguments, cont.

SPECIFIER	ARGUMENTS	FORMAT	DESCRIPTION example
ndf	ksect,ndfname	i, a72	read section ksect from PENDF file ndfname `ndf 102,mypendftape`
npt	kpts, keres,kgamr	i 2i	0=histogram, 1=dots, 20(21)=small(big) circles >0 says write res. Energies, Widths `npt 1,0,0`
nrm	Anorm(1-8)	8f	Normalize data File i by Anorm(i) `nrm  1.0,2.4,0.76,8.25`
nxy	nx,ny,kstack	3i	# x frames, # y frames, # plots stacked, `nxy 1,2,1`
odf	odfname *	a72 a1	ODF file name : $\leq$ 72 characters Reads up to 8 ODF files in current directory `odf /home/xyz/u235/total.odf`

ops	nx,ny,kstack,
	kpts,
	keres,kgamr
		6i	# x frames, # y frames, # plots stacked,
			0=histogram, 1=dots, 20(21)=small(big) circles
			>0 says write resonance energies, widths
			`ops  1 1 2 1 1 1`

ovr	kover	i	Overlay kover plots in 1 window (kover <9) `ovr 2`
oxp	oxp_string	a72	String for plot request specifier Default: `oxp 1 dtb`
oxs	oxs_string	a72	String for plot request - plot stays on screen `oxs 1 etb 210.,290.`
pan	xp, xpwid, xpmax	3f	plot from xp to xpmax in steps of 2*xpwid `pan 200.,50.,700.`
par	inparfile	a72	PAR file name : $\leq$ 72 characters `par my_par_file_name`
pkr	temp, dist, deltal, deltae, deltag, crfn, thick	7f	set SAMMY parameters for Peak Fitting `pkr 300.,201.3,.012,.005,.01,5.35,1.1`
pks	fwhm, bias, a2targ, itarg, jtot, gamgam, fwhmax	7f	see section on Peak Search and Fitting `pks 1.1,3.0, 235.,0.,0.5,0.5,1.2`
plt	pltname *	a72 a1	PLT file name : $\leq$ 72 characters Reads up to 8 PLT files in current directory `plt /home/xyz/u235/total.plt`
q			tells RSAP to quit.
rat	kratout	i	>0 says write values to file "rsap.ratexpth"
sam			run SAMMY using PAR file rsap.peaks
sgb	ksgvbestchi	i	set # of "best chi" SGV values to plot `sgb 4`
sgd	sgd_name	a72	SAMMY data file name: $\leq$ 72 characters `sgd my_SAMMY_data_file_name`
sgi	sgi_name	a72	SAMMY input file name: $\leq$ 72 characters `sgi my_SAMMY_input_file_name`
sgr	numres, jsg1, , jsg8	9i	SGV resonance number, spin group list `sgr  25, 4, 5, 6`

Table 2. RSAP Specifiers and Arguments, cont.

SPECIFIER	ARGUMENTS	FORMAT	DESCRIPTION example
sgv	esglo, esghi	2f	min and max energies for SGV fit `sgv  380.,430.`
sgp			Automatic plot of SGV fit results
stk	kstack	i	number of plots to stack `stk 5`
sym	ksymodf(1-8)	8i	ksymodf(i) = symbol for data file i `sym 1,20,21,0,22`
sys	command	a72	execute Unix "command" `sys mv oldname newname`
thn	kthin, elo, ehi	i,2f	thin data file between elo and ehi `thn 4,2000.,3000.`
tit	title_string	a32	32-character title string `tit my plot title`
txt	kt, ktcol, xt,yt, sizet, angle, txtstring	2i 4f a40	data file #, text color, position (xt, yt), size, angle, 40-character text string `txt  1,9,250.3,200.,2.0,,MyText`
typ	kodf, elo, ehi	i,2f	type values from file kodf between elo and ehi `typ 1 : types first 3 values from data file 1`
una	scale, numwids	2f	auto no Bayes fits, SAMMY.PUB uncertainties `una 3.,5.`
unc	elo, ehi	2f	no Bayes fits, elo to ehi in eV `unc 4500.,4800.`
unp	iview, iprint	2i	set parameters for una `unp 3`
unr	i1,i2,...	8i	set resonance numbers for una and unc `unr 25, 26, 27`
unt	itype	i	1,2,3,4 : capture,neutron,fission1, fission2 widths `unt 2`
unw	iw1, iw2,...	8i	una width scale factors in percent `unw 90, 100, 110`
uni	icode, elo, ehi	i,2f	union energy grid between elo and ehi `uni 2, 100.,400.`
xlb	xaxlabel	a24	24-character X-axis label `xlb my X-axis label`
ylb	yaxlabel	a24	24-character Y-axis label `ylb my Y-axis label`
x ps psc			output to X-window, rsap.ps, rsap.psc, rsap.meta output to file rsap.ps output to file rsap.psc
###			Comment - ignored by RSAP

5 Example Input Files

Several sample RSAP input files are described in this section. Each example corresponds to one of the sample plots displayed in Figures 1-11. The **exa** specifier may be used to obtain a list of examples, to type the contents of an example input file, or to run a particular example and plot :

```
rsap
RSAP6> ###       type list of examples
RSAP6> exa
RSAP6> ###       type input file for example 4
RSAP6> exa 4
RSAP6> ###       run example 4 and plot
RSAP6> exa 4, plot
```

Note that the device specifier "**x**" sends the plot to four devices: an X plot window, a PLPLOT metafile **rsap.meta**, the color postscript file **rsap.psc**, and the monochrome postscript file **rsap.ps**. The postscript files may then be sent to the default printer:

"**lpr -h rsap.ps**" or "**lpr -h rsap.psc**".

A postscript file may be viewed via "**ghostview -seascape rsap.psc**".

A postscript file may be created without plotting to an X window by replacing the specifier "**x**" with "**ps**" or "**psc**".

5.1 Example 1. One Plot in One Window

This input compares the input par file **JohnFowl235_990203.par** with the final SAMMY parameter file **SAMMY.PAR**, reads **JohnFowl235_990203.odf**, and plots one frame (nxp=nyp=1) to an X window. The "**deb**" card specifies a plot of cross section data with error bars and the Bayes fit for 2200 < E < 2500 keV with y-axis limits of 0 and 1.0 b. If axis limits are not specified, the plot will span the range of data values. Resonance energies and widths are displayed (keres=1, kgamres=1) on the plot. A blank card ends the input for this particular plot sequence and causes the plot to be drawn on the output device. The "q" in column 1 tells RSAP to quit. The "###" comment card is ignored by the code.

```
par /home/ros/RSAP/EX/1/JohnFowl235_990203.par     (a4,a72)
odf /home/ros/RSAP/EX/1/JohnFowl235_990203.odf     (a4,a72)
tit JohnFowl235_990203 3.784                       (a4,a32)
###  # x frames,  # y frames,  # plots stacked
nxy 1,1,1
###   (kpts = 0,1,20,21 says histogram, dots, circles, big circles)
###  kpts, keres,kgres
npt 1 1 1
x            output device    (x  , ps, psc)
1 deb 2200.,2500.,0.0,1.0                        (a2,a4,4f)

q
```

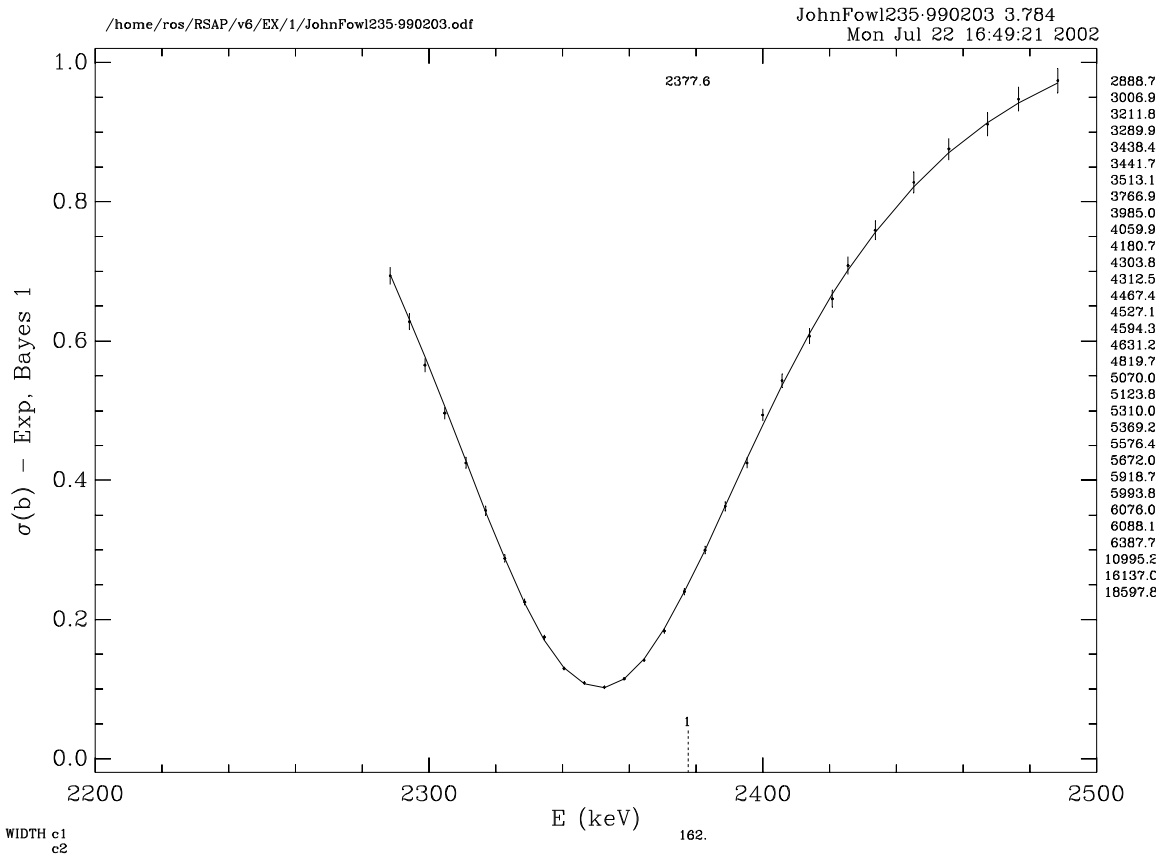


Figure 1: /home/ros/RSAP/EX/1/inx

To make this plot on your X terminal, type at the RSAP prompt: "RSAP6> exa 1,plot"

You should see a plot like the one in Figure 1. On your screen the background should be black. After RSAP reads the "**deb**" card and sends the plot to your screen, the code waits for a "RETURN" before reading the next input record. Alternatively, the "**x**" and "**1 deb**" cards could be replaced by one "**oxp**" record:

```
oxp 1 deb 2200.,2500.,0.0,1.0                    (a4,a2,a4,4f)
```

The "`par`", "`tit`", "`nxy`", and "`npt`" specifiers are optional. The default "`nxy`" and "`npt`" arguments are:

```
nxp=nyp=1        (1 frame in x direction, 1 frame in y direction)
kstack=1         (1 plot per frame)
kpts=0           (plot data as histograms)
keres=kgres=0    (no display of resonance energies, widths)
```

Above the plot the ODF file name, title, date, and time are listed. If the SAMMY output file SAMMY.LPT exists, the conventional CHISQ/NDAT is also listed above the plot. If keres=1, spin group numbers are listed just above the bottom x axis, and resonance energies are listed just below the top x axis. Resonance energies greater than the x-axis maximum are listed to the right of the plot.

5.2 Example 2. Stack 2 plots in 1 window

To see an example of stacking 2 plots in a window (Figure 2) , type:

```
rsap
RSAP6>exa 2,plot
```

```
par /home/ros/RSAP/EX/2/bcjav3ndsh_990203.par
odf /home/ros/RSAP/EX/2/bcjav3ndsh_990203.odf
tit cjav3/C 990203 3.78, 6.5            Title (a32)
###  number of x frames, y frames, plots stacked
nxy 1,1,2
###   (kpts = 0,1,20,21 : histogram, dot, circle, big circle)
###  kpts, keres,kgres
npt 1 1 1
x
1 dtb 4000.,4700.,0.5,3.5
1 rb  4000.,4700.
q
```

The upper plot in Figure 2 shows both the residuals (dots) and the Bayes fit.

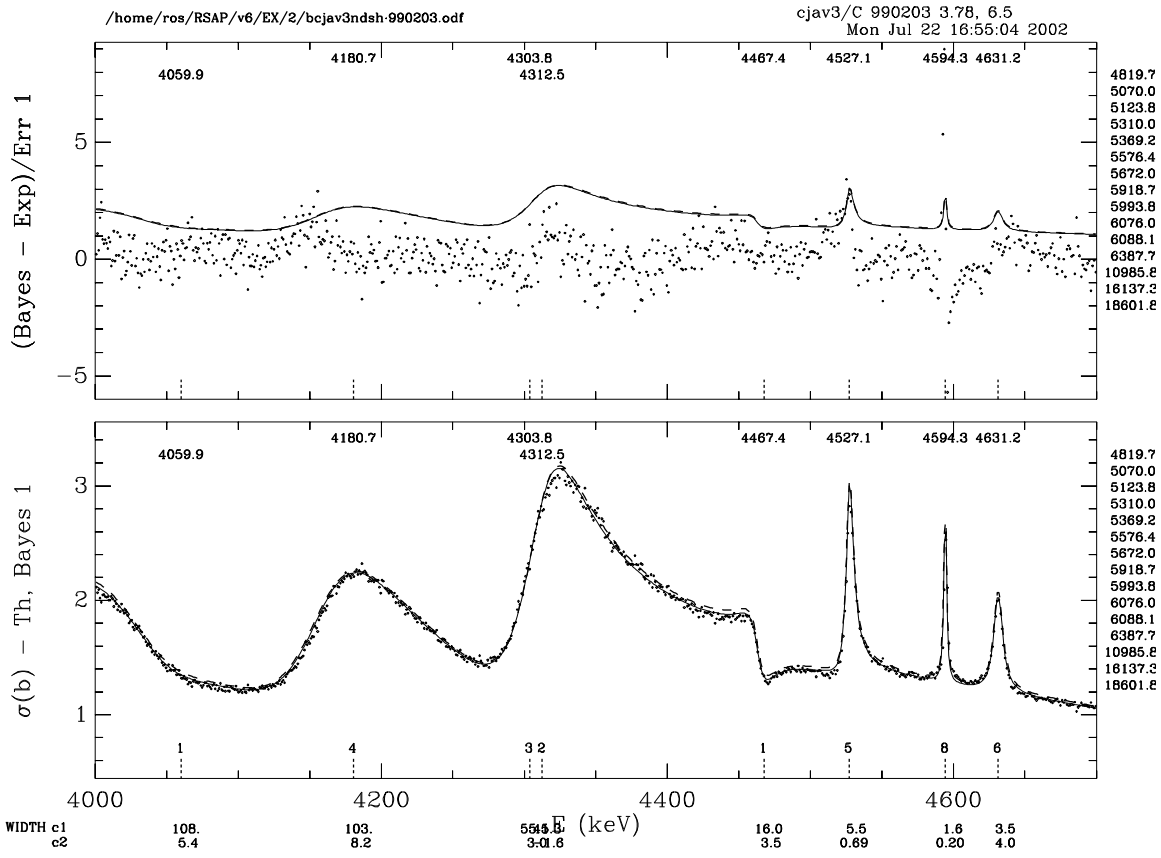


Figure 2: /home/ros/RSAP/EX/2/inx

5.3 Example 3. Plot from 2 ODF files

Plots from two ODF files may be stacked in one window:

```
RSAP6>exa 3,plot
```

```
par /home/ros/RSAP/EX/3/JohnFowl235_990203.par
odf /home/ros/RSAP/EX/3/JohnFowl235_990203.odf
odf /home/ros/RSAP/EX/3/duanesh_990203.odf
tit 990203.   JohnFowl235 + duanesh
###  number of x frames, y frames, plots stacked
nxy 1,1,2
###  (kpts = 0,1,20,21 : histogram, dot, circle, big circle)
###  kpts, keres,kgres
npt 0,1,1
x
1 deb 2250.,2450.,0.0,0.80                    (i2,a3, 4f)
2 dtb 2250.,2450.,0.0,1.5
```

Note that the code will terminate properly when the end of the input file is reached.

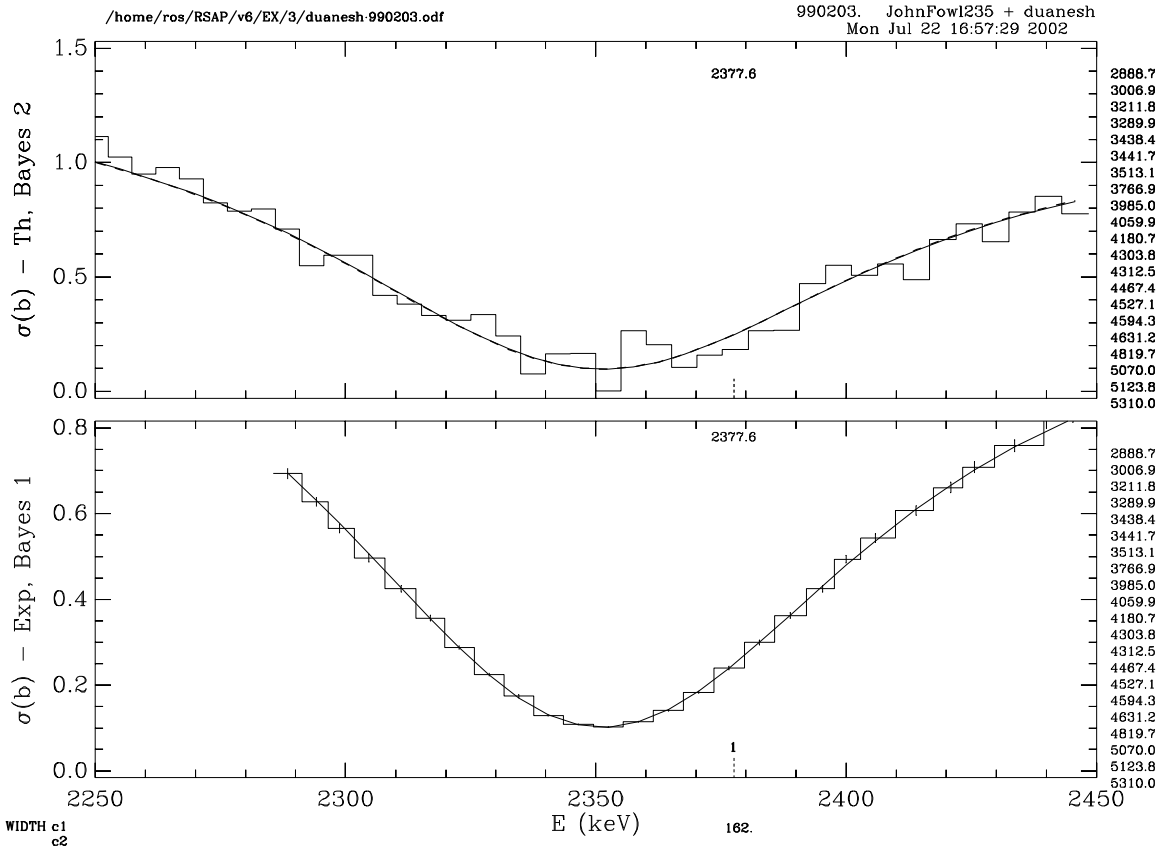


Figure 3: /home/ros/RSAP/EX/3/inxs2

5.4 Example 4. Transmission plots

Transmission data may be displayed by plot requests that begin with "a" or "b" instead of "1" or "2" as shown in the following sample input. Transmission ("a det 0.,400.,0.0,1.0") and total cross section data ("1 det 0.,400.") from the first ODF file are stacked in the upper frame in an X plot window (see Fig. 4), and the corresponding quantities for the second ODF file are stacked in the lower frame. Note that the **lpr** specifier automatically sends the monochrome postscript file **rsap.ps** to the default printer.

```
odf /home/ros/RSAP/EX/4/bal27orthin_990309.odf
odf /home/ros/RSAP/EX/4/bal27orthick_990309.odf
tit Al27 ORELA thin,thick. AV 5
avg 5
###     red for theory, blue for bayes, green for data
col r b g
### number of x frames, y frames, plots stacked
nxy 1,2,2
### plot data as dots
npt 1
fnt 2
x
a det 0.,400.,0.0,1.0
1 det 0.,400.,0.,40.
b det 0.,400.,0.0,1.0
2 det 0.,400.,0.,40.

lpr
q
```

To make the above plots on your X terminal (see Fig. 4) , type:

```
rsap
RSAP6 > exa 4,plot
```

In this example the plot contains the text "**< 5>**" at the top of the frame, indicating that 5 data points were averaged before plotting.

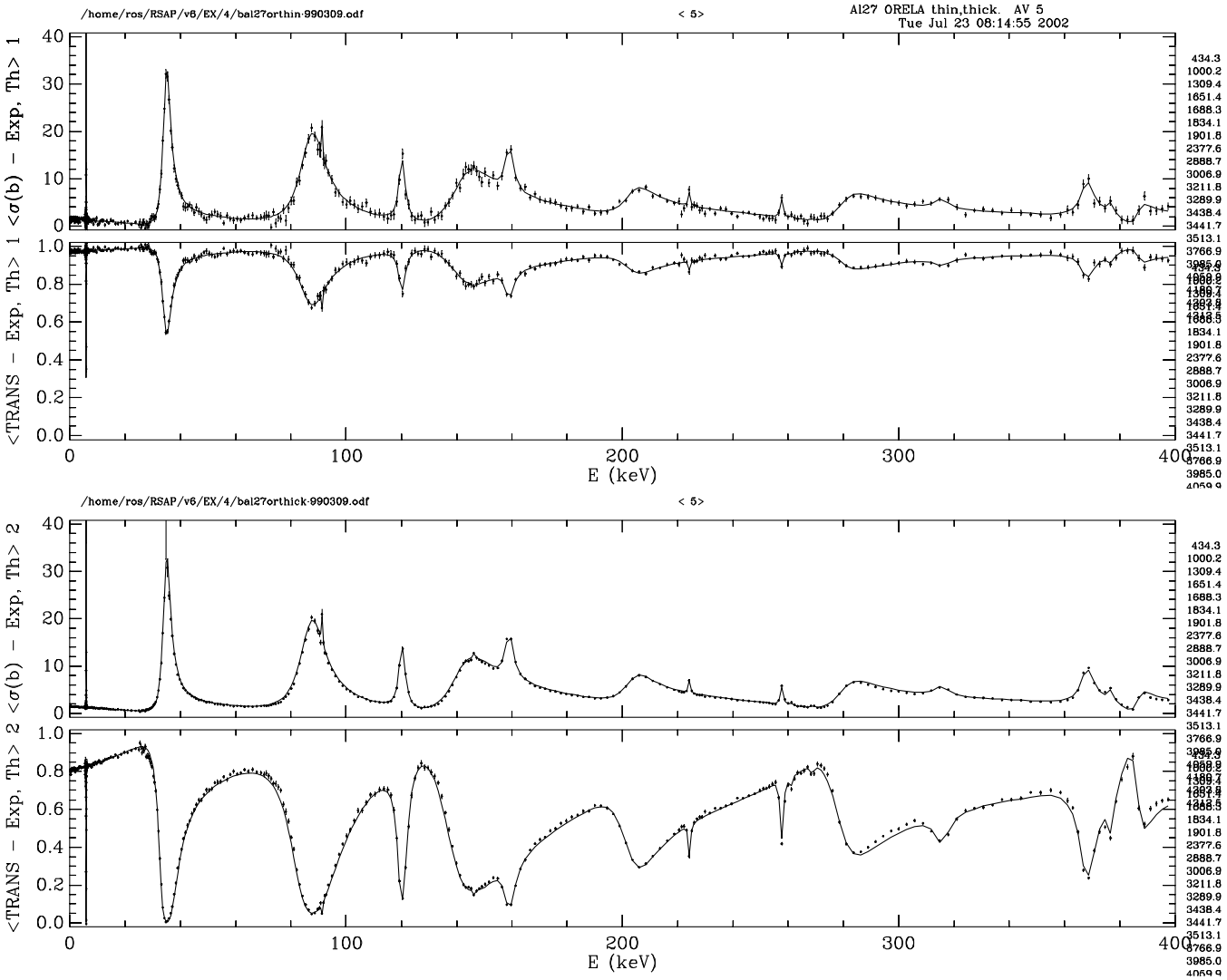


Figure 4: /home/ros/RSAP/EX/4/alortrantot

5.5 Example 5. Colors

Colors for data, theory, and bayes may be set with the `col` specifier:

```
### set theory to yellow, bayes to red, data to yellow for all plots
col y r g
### set theory to blue, bayes to magenta, data to cyan for all plots
col b m c
```

To see an example for the `col` specifier, type: `rsap < /home/ros/RSAP/EX/5/incolxpsc` .

More flexibility is obtained with the `cst` specifier, which allows different color combinations for different data files. For example:

```
### set colors for odf file 1, 2, 3, 4
cst data   green  magenta salmon wheat
cst theory yellow blue    brown   turquoise
cst bayes  red    cyan    aqua    blueviolet
```

To see a plot illustrating the above commands, type "`exa 5,plot` "at the RSAP prompt.

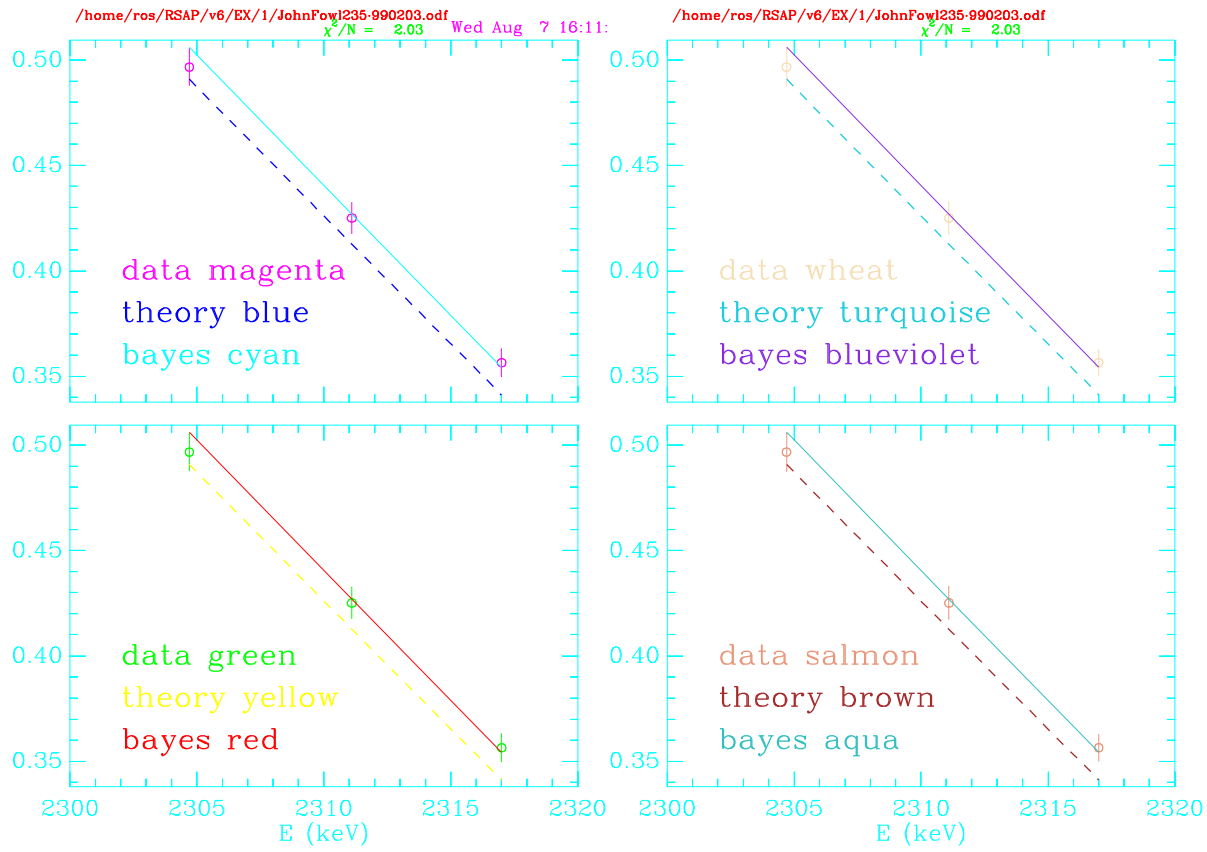


Figure 5: /home/ros/RSAP/EX/5/incst

5.6 Example 6. Figure Captions

A 64-character figure caption string may be written at the bottom edge of the plot window with the **cap** specifier. Vertical axes are scaled to fit plots and caption in the window. Figure captions are supported for the case of one plot per page in the x-direction (`nxy 1`). An example is given in Fig. 6, which was produced by the file `/home/ros/RSAP/EX/6/incap` :

```
par /home/ros/RSAP/EX/1/JohnFowl235_990203.par
odf /home/ros/RSAP/EX/2/bcjav3ndsh_990203.odf
###        number of x frames, y frames, plots stacked
nxy 1,1,1
###   (kpts = 0,1,20,21: histogram, dot, circle, big circle)
###  kpts, keres,kgres
npt 1 1 0
cap Here is an  example of a figure caption
###         Roman font
fnt 2
x
1 dtb 4100.,4700.,0.5,3.5

q
```

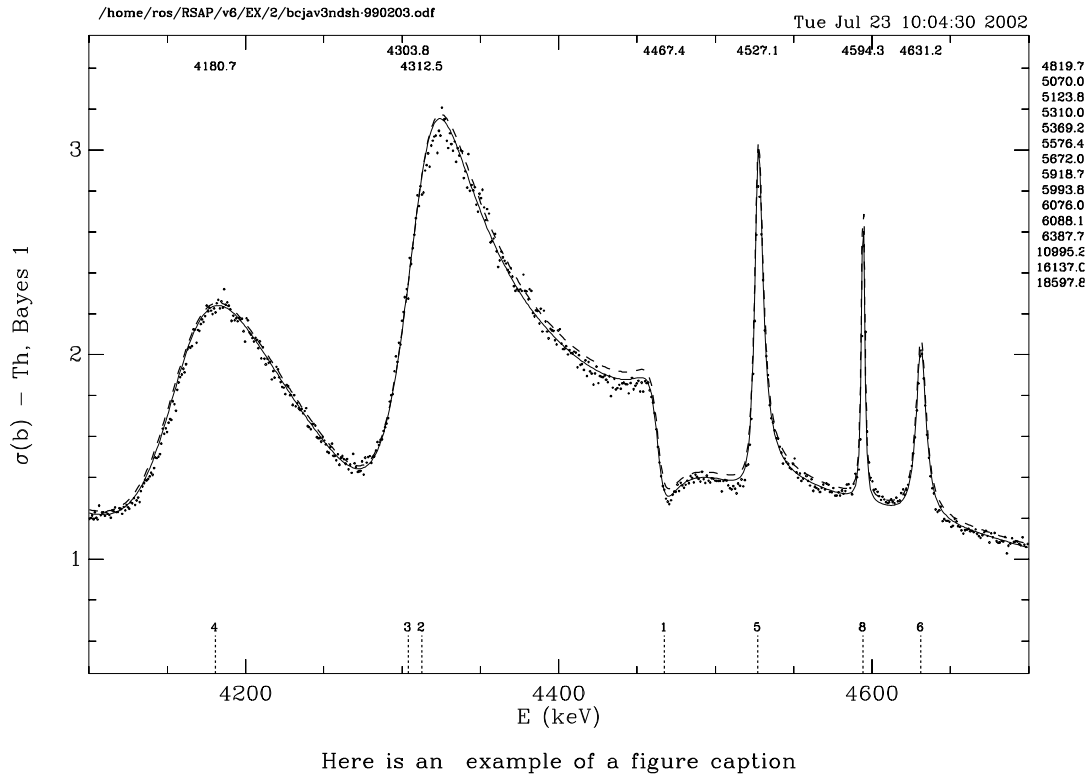


Figure 6: /home/ros/RSAP/EX/6/incap

5.7 Example 7. Plotting from 3 ODF Files and Annotation Strings

The **ann** specifier can be used to position a text string at the left (4), center (5), or right (6) of the plot. Plotting from 3 ODF files and annotation strings are illustrated in Fig. 7, which was produced by the command: `rsap < /home/ros/RSAP/EX/7/in3odf`

```
par /home/ros/RSAP/EX/7/JohnFowl235_990203.par
odf /home/ros/RSAP/EX/7/JohnFowl235_990203.odf
odf /home/ros/RSAP/EX/7/duanesh_990203.odf
odf /home/ros/RSAP/EX/7/FJF73lows6_990824.odf
tit Plot from 3 odf files
### odf#, pos, col, txtstring (a4, i1, i1, i2, a40)
ann 14  PLOT 1 JohnFowl235. Position 4
ann 25  PLOT 2 duanesh. Position 5.
ann 36  PLOT 3 FJF73lows6.  Position 6
###        number of x frames, y frames, plots stacked
nxy 1,1,3
###   (kpts = 0,1,20,21: histogram, dot, circle, big circle)
###  kpts, keres,kgres
npt 1 0 0
###
x
1 etb 2250.,2450.,0.0,0.80
2 etb 2250.,2450.,0.0,1.5
3 det 2250.,2450.,0.0,1.5

q
```

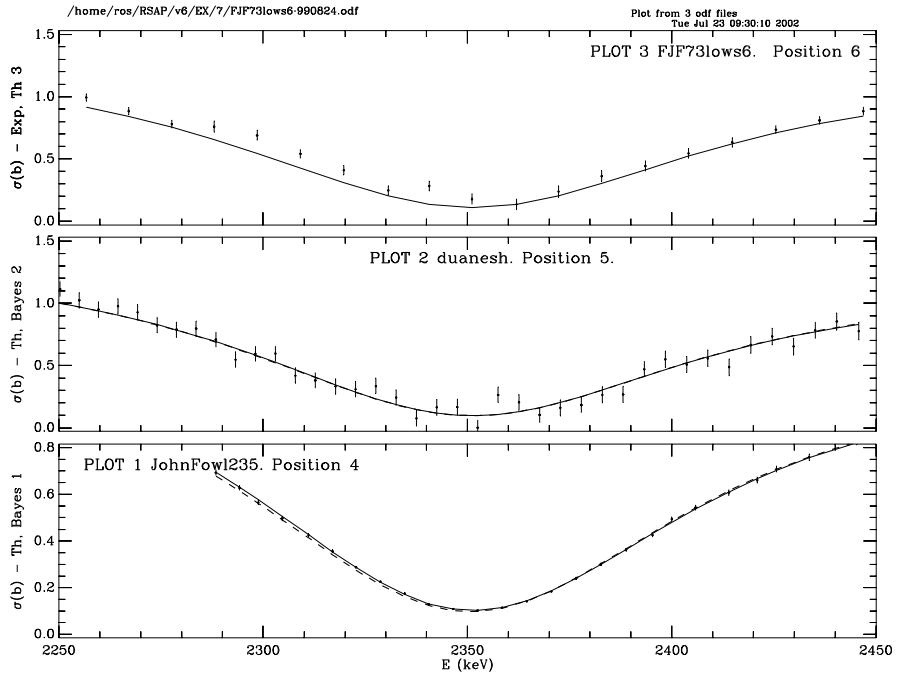


Figure 7: /home/ros/RSAP/EX/7/in3odf

5.8 Example 8. Place 6 Plots in 1 Window

To put plots from 6 ODF files in a single window in a 2x3 xy matrix and send the file **rsap.ps** to the default printer:

```
/home/ros/RSAP/EX/8/inpl_231

     par /home/ros/RSAP/EX/8/FJF73lows6_991005.par
     odf /home/ros/RSAP/EX/8/DROTnob_991005.odf
     odf /home/ros/RSAP/EX/8/bBH_aftercj_991005.odf
     odf /home/ros/RSAP/EX/8/bcjav3ndsh_afterBH_991005.odf
     odf /home/ros/RSAP/EX/8/FJF73lows6_991005.odf
     odf /home/ros/RSAP/EX/8/JohnFowl235_991005.odf
     odf /home/ros/RSAP/EX/8/duanesh_991005.odf
     tit Plot from 6 odf files
     ###    odf#, pos, col, txtstring         (a4, i1, i1, i2, a40)
     ann 15  PLOT 1 DROTnob_991005 POS 5
     ann 25  PLOT 2 bBH_aftercj_991005 POS 5.
     ann 35  PLOT 3 bcjav3ndsh_afterBH_991005  POS 5
     ann 45  PLOT 4 FJF73lows6_991005 POS 5
     ann 55  PLOT 5 JohnFowl235_991005 POS 5.
     ann 65  PLOT 6 duanesh_991005  POS 5
     ###        number of x frames, y frames, plots stacked
     nxy 2,3,1
     ###   (kpts = 0,1,20,21: histogram, dot, circle, big circle)
     ###  kpts, keres,kgres
     npt 1 0 0
     x
     1 etb 3200.,4000.
     2 etb 3200.,4000.
     3 det 3200.,4000.
     4 etb 2250.,2450.,0.0,1.5
     5 etb 2250.,2450.,0.0,0.80
     6 det 2250.,2450.,0.0,1.5

     lpr
     q
```

Other sample input files in the **EX/8** directory will plot in a 3x2 xy matrix (`in6odf_321`), and in a 6x1 xy matrix (`in6odf_stack6`).

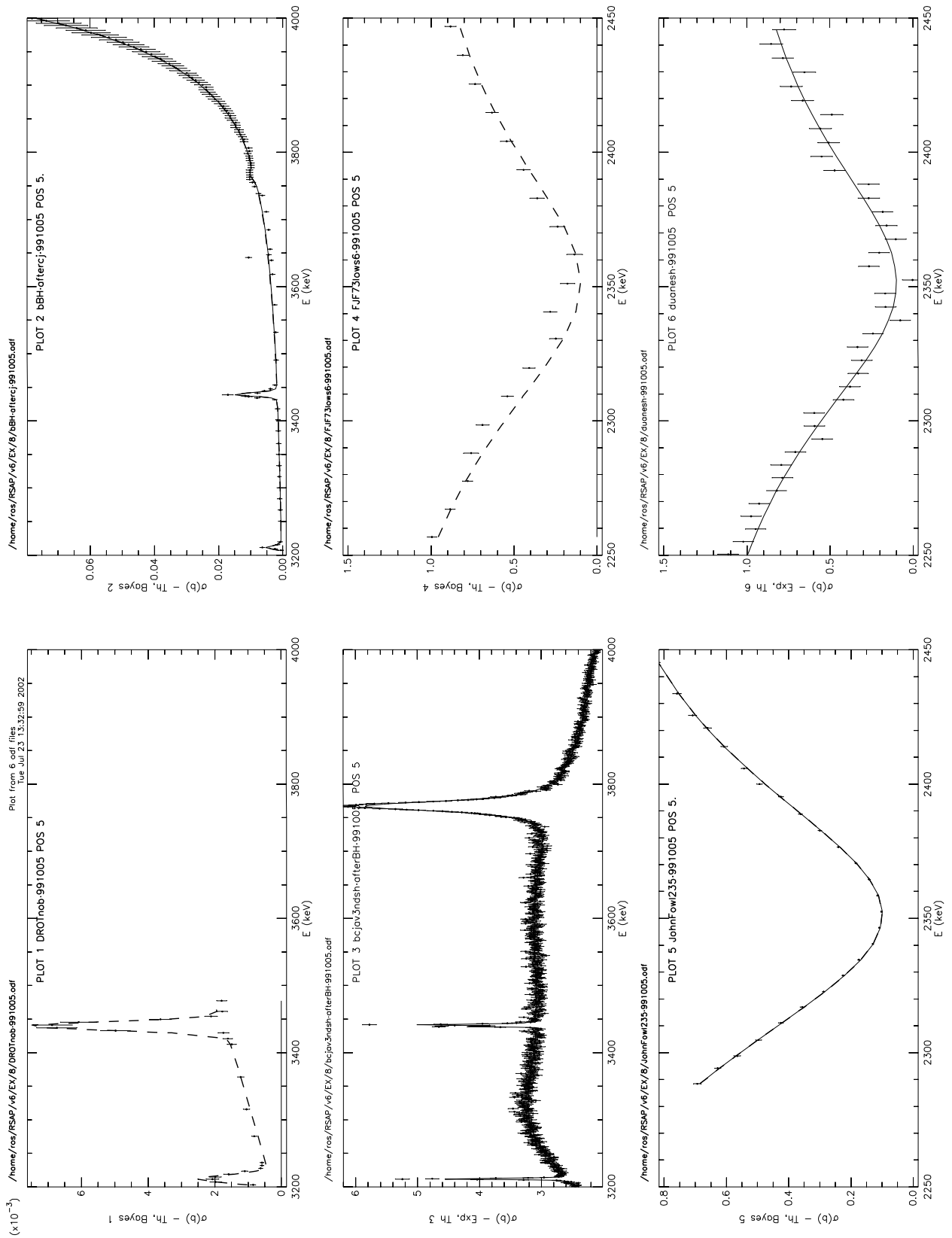


Figure 8: /home/ros/RSAP/EX/8/inpl_231

5.9 Example 9. Overlay 6 Plots in 1 Window

The number of plots to be overlaid is determined by the **ovr** specifier. To overlay plots from 6 ODF files in a window (see Fig. 9) :

```
rsap < /home/ros/RSAP/EX/9/inovr6

     par /home/ros/RSAP/EX/8/FJF73lows6_991005.par
     odf /home/ros/RSAP/EX/8/DROTnob_991005.odf
     odf /home/ros/RSAP/EX/8/bBH_aftercj_991005.odf
     odf /home/ros/RSAP/EX/8/bcjav3ndsh_afterBH_991005.odf
     odf /home/ros/RSAP/EX/8/FJF73lows6_991005.odf
     odf /home/ros/RSAP/EX/8/JohnFowl235_991005.odf
     odf /home/ros/RSAP/EX/8/duanesh_991005.odf
     tit RSAP v.6.  OVERLAY 6 odf files
     ### omit odf name, write date, omit CHISQ/N
     lab  0 1 0
     ylb  Cross Section in barns
     ovr  6
     ###  Normalization factors for odf files 1 - 6.
     nrm  1.0,1.0,3.0,0.2,10.,1.
     log  0 1
     ###  Roman Font
     fnt  2
     ###        number of x frames, y frames, plots stacked
     nxy 1,1,1
     ###   (kpts = 0,1,20,21: histogram, dot, circle, big circle)
     ###  kpts, keres,kgres
     npt 1 0 0
     x
     1 etb 0000.,6300.,0.02,20.
     2 etb 3200.,4000.
     3 det 3200.,4000.
     4 etb 2250.,2450.
     5 etb 2250.,2450.
     6 det 2250.,2450.

     q
```

Normalization factors were applied to each plot with the **nrm** specifier, and the **lab** specifier was used to inhibit output of the odf name and CHISQ/NDAT to the plot.

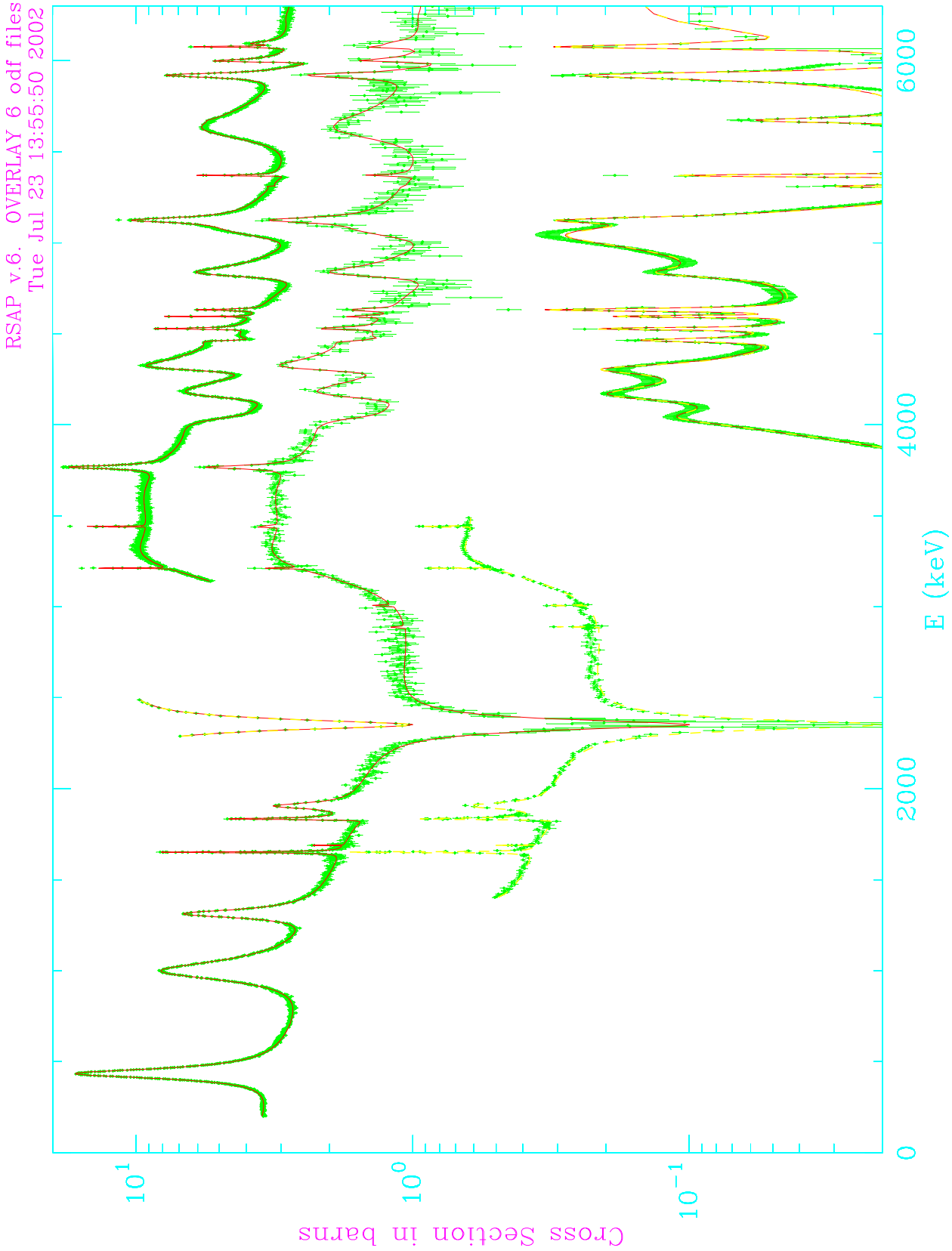


Figure 9: /home/ros/RSAP/EX/9/inovr6

5.10 Example 10. Text Strings using txt

Text strings may be written at user (x,y) locations with the **txt** specifier. String size, orientation, and color may be specified as illustrated in Fig. 10, which was produced by the file :

```
/home/ros/RSAP/EX/10/intxt

     ev  2
     log 0,0
     odf /home/ros/RSAP/EX/5/233b10trn.odf
     odf /home/ros/RSAP/EX/5/233b10trn.odf
     odf /home/ros/RSAP/EX/5/233b10trn.odf
     odf /home/ros/RSAP/EX/5/233b10trn.odf
     odf /home/ros/RSAP/EX/5/233b10trn.odf
     odf /home/ros/RSAP/EX/5/233b10trn.odf
     ###        2 frames in x, 1 frame in y, stack 3
     nxy 2,1,3
     npt 1
     tit  text string test
     lab
     ###  Roman font
     fnt 2
     ###  red yellow green blue cyan magenta white
     ###    1      2     3    9   11      13    15
     ###
     ### nodf,col, xt, yt, sizet, angle, string (2i, 4f, a40)
     txt  1, 9, 250.3, 200., 2.0, ,Double Size-------20--------30
     txt  2, 3, 250.5, 220., 1.0, ,Normal Size-------20--------30--------40
     txt  3, 1, 251.,  200., 0.5, ,Half Size---------20--------30--------40
     txt  4,13, 250.5, 200., 1.0,-45.,****TEXT STRING AT -45 DEGREES****
     txt  5,13, 250.4,  20., 1.1, 45.,****TEXT STRING AT  45 DEGREES****
     txt  6,13, 251.,   10., 0.9, 90.,****TEXT AT 90 DEGREES****
     x
     1 db  250.0,255.,0.0,250.
     2 db  250.0,255.,0.0,250.
     3 db  250.0,255.,0.0,250.
     4 db  250.0,255.,0.0,250.
     5 db  250.0,255.,0.0,250.
     6 db  250.0,255.,0.0,250.

     sys mv rsap.psc rsaptxt.psc
     q
```

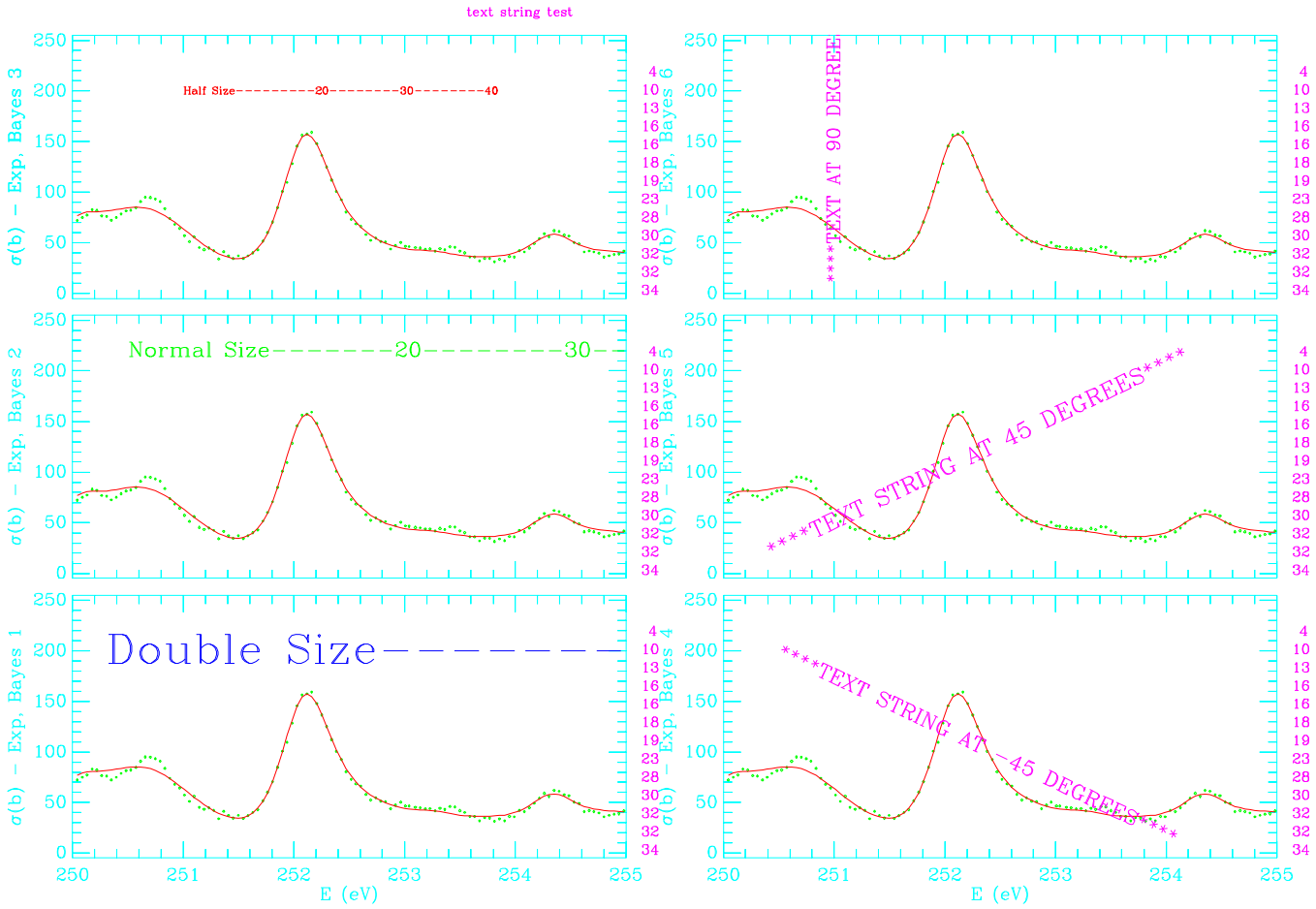


Figure 10: /home/ros/RSAP/EX/10/intxt

5.11 Histogram Dash Patterns

By default data is plotted in histogram mode (npts = 0) as solid lines. Other line patterns may be chosen with the **dsh** specifier. Eight different dash patterns are set for data files 1 through 8 with the specifier:

```
dsh  1,2,3,4,-3,-5,-7,-9
```

To see these patterns:

```
rsap < /home/ros/RSAP/EX/14/dodsh
```

Normally the "theory" is plotted as lines connecting values at the energies in the data file. However, it is possible to plot both data and theory as histograms as shown in the example:

```
rsap < /home/ros/RSAP/EX/14/dohis
```

5.12 Scaling of Axis Labels

When preparing figures for publication, it is often desirable to increase the size of labels. Axis labels may be scaled by a factor input as the second argument of the fnt specifer. To specify Roman font and scale axis labels by a factor 1.5

```
fnt 2,1.5
```

To plot an example illustrating axis label scaling on your X terminal (see Fig. 11) , type:

```
rsap
RSAP6 > exa 16,plot
```

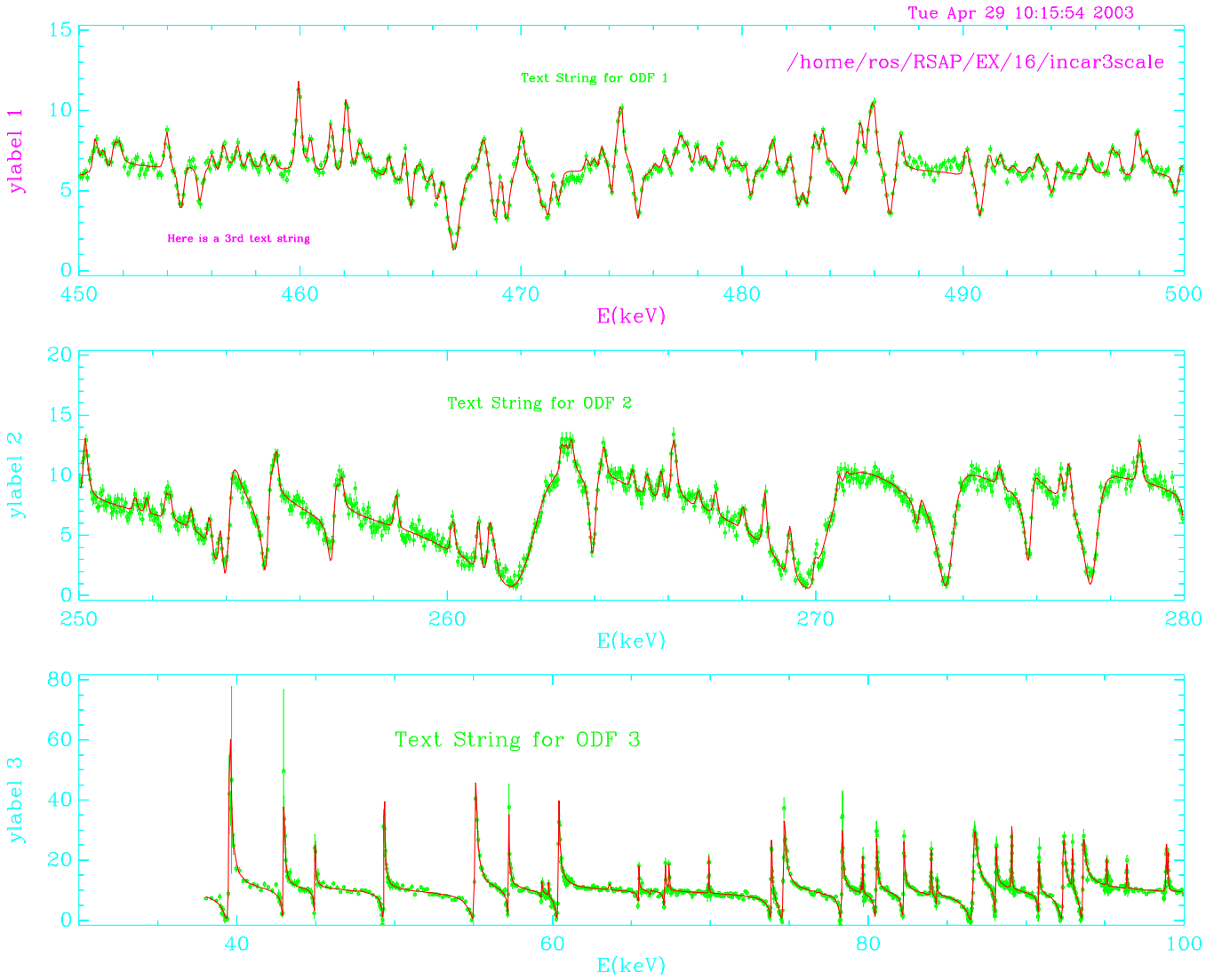


Figure 11: /home/ros/RSAP/EX/16/incar3scale

6 Peak Search and Fitting

A peak search procedure has been implemented in RSAP to provide an initial PAR file for use with SAMMY. The procedure, an adaptation of the method of Mariscotti [5], is based on computation of the second derivative of the data averaged over a width parameter, **fwhm**. A second parameter, **bias**, is approximately the number of standard deviations above background for a peak to be found. A peak search is requested with the "`pks`" specifier.

```
pks fwhm, bias, a2targ, itarg, jtot, gamgam, fwhmax
```

where **fwhm** is the full width at half-maximum (FWHM) in eV, **bias** is the sensitivity parameter, **a2targ** is the mass number of the target, **itarg** is the target spin (I), **jtot** is the total spin (J), **gamgam** is the capture width in eV (default 1.0), and **fwhmax** is the maximum value in eV allowed for the FWHM of a peak.

RSAP searches for peaks in the total cross section data in the energy range specified and estimates the width, height, and area of each peak found. The data and a sum of SLBW (single-level Breit-Wigner) shapes are then plotted. RSAP writes an output file, **rsap.peaks**, containing a list of energy, gamma width Γ_γ, neutron width Γ_n, fission widths, and flags in the format of the SAMMY PARameter file. Estimates of the peak height σ_o, total width Γ, statistical factor g, and wave number k, are used to estimate Γ_n and the fission width, Γ_f .

$$\begin{aligned} 4\pi g\Gamma_n &= \sigma_o k^2 \Gamma \\ \Gamma_f &= \Gamma - \Gamma_\gamma - \Gamma_n \end{aligned}$$

After a peak search, the "`sam`" specifier will tell RSAP to create a SAMMY input file, **rsap.samin**, do a SAMMY Bayes run with the input PAR file **rsap.peaks** , and plot the results. An example input file, `/home/ros/RSAP/EX/11/tranxps`, is reproduced below.

```
ev   2
log  0 0
odf /home/ros/RSAP/EX/11/u233temp.odf
tit PKFIND FWHM 1.1, BIAS 3.
nxy 1,1,1
npt 0,1,1
### fwhm, bias, a2targ, spintarg, spintot, gamgam, fwhmax
pks 1.1, 3.0, 235., 0.,0.5, 0.5, 1.2
x
1 etb  500.,516.,0.0,70.

sam
q
```

On the upper plot of Fig. 12 the solid line is the sum of SLBW shapes, and the dashed line is the SLBW sum plus a linear background computed from the first and last data points. On the lower plot of Fig. 12 the solid line is the SAMMY Bayes fit, and the dashed line is the SAMMY theory (initial theoretical value).

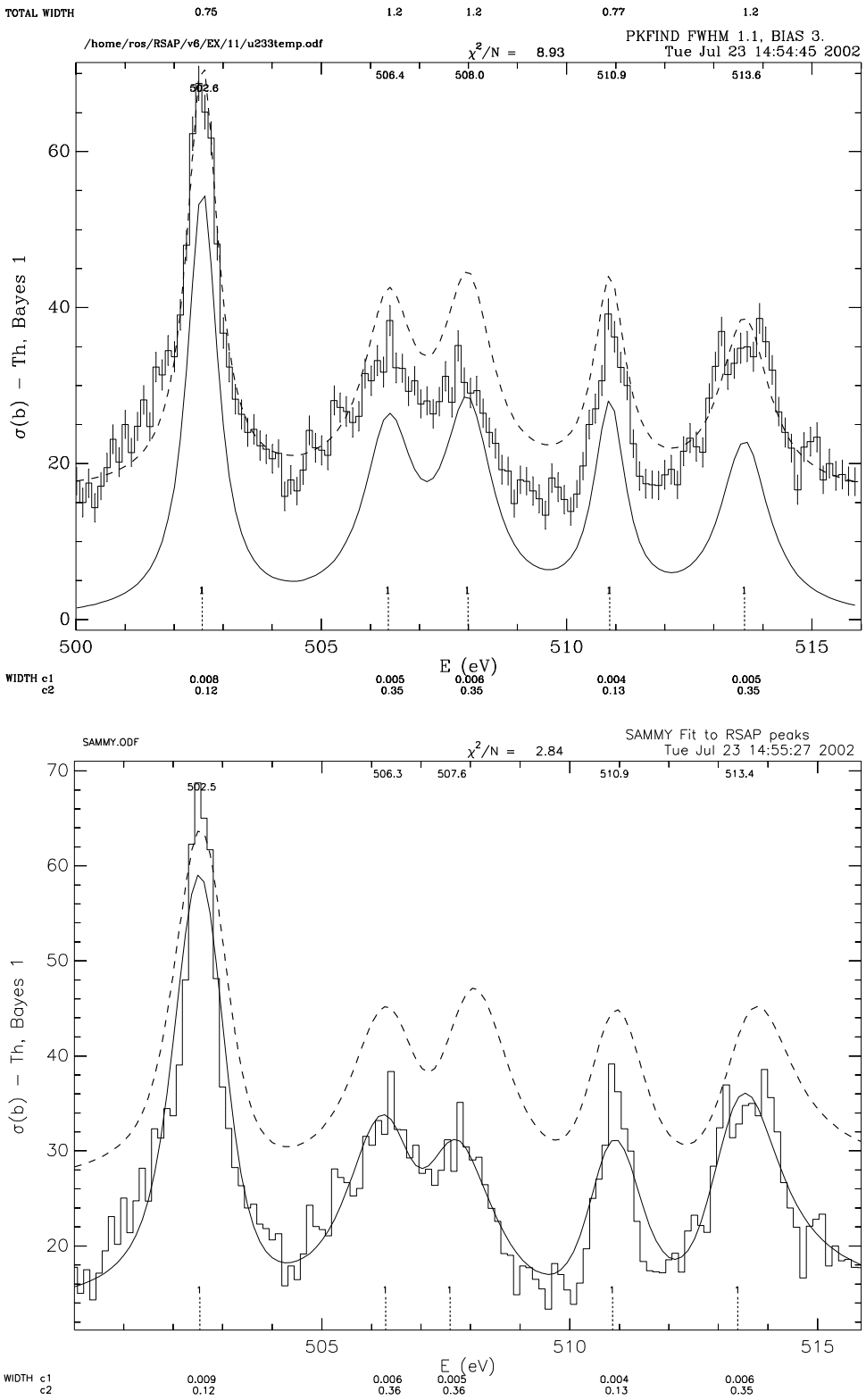


Figure 12: /home/ros/RSAP/EX/11/tranxps. Upper plot: sum of SLBW shapes (solid); SLBW sum plus a linear background (dashed). Lower plot: SAMMY Bayes fit (solid); SAMMY initial theoretical value (dashed).

For particular cases much improved search and fit results can be obtained by setting the fission widths to zero (`fis` specifier) and/or setting the SAMMY resolution parameters (`pkr` specifier). Example 15 illlustrates the use of the `fis` and `pkr` specifiers for the ^{238}U total cross section in the range 10 keV $< E <$ 11 keV. As shown in Fig. 13, 28 peaks were found and a good SAMMY fit was obtained with the input file /home/ros/RSAP/EX/15/fitu238:

```
ev   2
odf /home/ros/RSAP/EX/15/u8mres1.odf
###           (kpts = 0,1,20,21: histogram, dot, circle, big circle)
###  kpts, keres,kgres
npt 0,1,1
###      set fission widths to zero
fis
### TEMP, flpath(m), DELTAL,DELTAE,DELTAG,CRFN,THICK
pkr  300.,201.558, 0.024, 0.0, 0.015, 9.43, 0.01235
###
### fwhm, bias, a2targ, Itarg, Jtot, gamgam, fwhmax
pks 4.5, 3.0, 238., 0., 0.5, 0.023, 5.0
x
1 etb  10000.,11000.,0.0,70.

sam
q
```

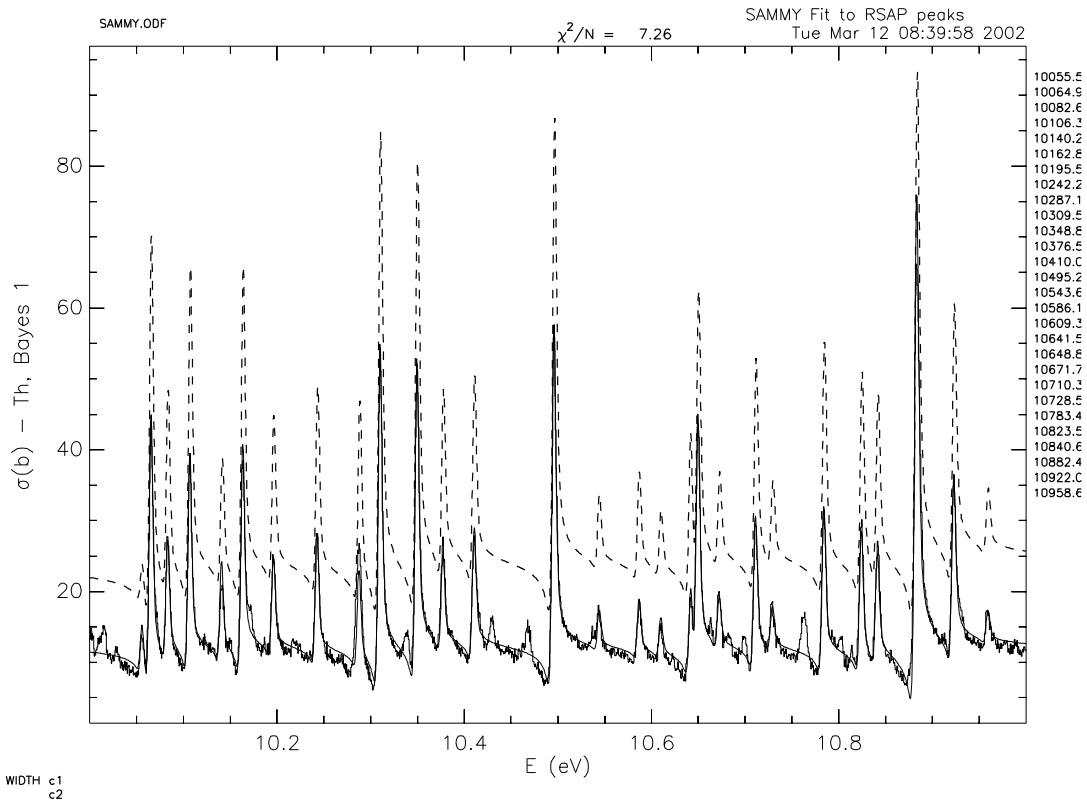


Figure 13: /home/ros/RSAP/EX/15/fitu238. SAMMY Bayes fit (solid); SAMMY initial theoretical value (dashed) based on RSAP peak search.

7 Automatic Spin Group Variation (SGV)

The process of fitting neutron cross section data with SAMMY often requires one to try several spin values in order to obtain the best fit for a given resonance or group of neighboring resonances. Each trial requires several steps: a) editing the PAR file to change the spin group number, b) running SAMMY, c) viewing the results, and d) comparison with results from other trials.

An automatic spin group variation (**SGV**) procedure has been implemented in RSAP to facilitate the determination of spin group values for resonances. A simple RSAP input file allows the user to specify SAMMY input and PAR files, one or more resonances, an energy range for the fit, and up to 8 spin groups for each resonance. For each specified spin group, RSAP automatically edits the PAR file, runs SAMMY, and writes out CHISQ/NDAT and final resonance parameters. The required specifiers and their arguments are :

```
par SAMMY_PAR_file_name
sgi SAMMY_input_file_name
sgd SAMMY_data_file_name
sgr resonance_number, jsg1, jsg2, ... , jsg8   (a4, 9i)
sgv esglo, esghi (a4, 2f)
```

The `resonance_number` corresponds to the record number in the PAR file, and `jsgi` is the spin group number to be used for the ith SAMMY fit. The action specifier **sgv** tells RSAP to loop over the indicated spin groups, fitting over the energy range (eV) from **esglo** to **esghi** . If a plot is wanted, the user should insert **sgp** after **sgv**. An example file with resonance 25 and spin groups 3, 5, and 6 is reproduced below.

`/home/ros/RSAP/EX/12/dosgv25`

```
par /home/ros/RSAP/EX/12/o16/FINAL326.par
### SAMMY input file
sgi /home/ros/RSAP/EX/12/o16/cjav3ndsh_M5.in
### SAMMY data file
sgd /home/ros/NUCDATA/sammy/o16/DATA/cj20742avg3normdsh.dat
### resonance number, spin group numbers
sgr 25, 3, 5, 6
### esglo, esghi
sgv 4500000., 4610000.
### automatic plot:
sgp
```

All parameters flagged in the user's original PAR file are varied in the SAMMY fits. RSAP does not modify the original PAR and INP files.

ODF and final PAR files for each spin group fit are saved in the subdirectory **000_00**, which is created by RSAP. A repeat SGV run causes **000_00** to be deleted and re-created. For the above example, the saved files are:

```
./000_00/SG_025_03.PAR ./000_00/SG_025_03.ODF
./000_00/SG_025_05.PAR ./000_00/SG_025_05.ODF
./000_00/SG_025_06.PAR ./000_00/SG_025_06.ODF
```

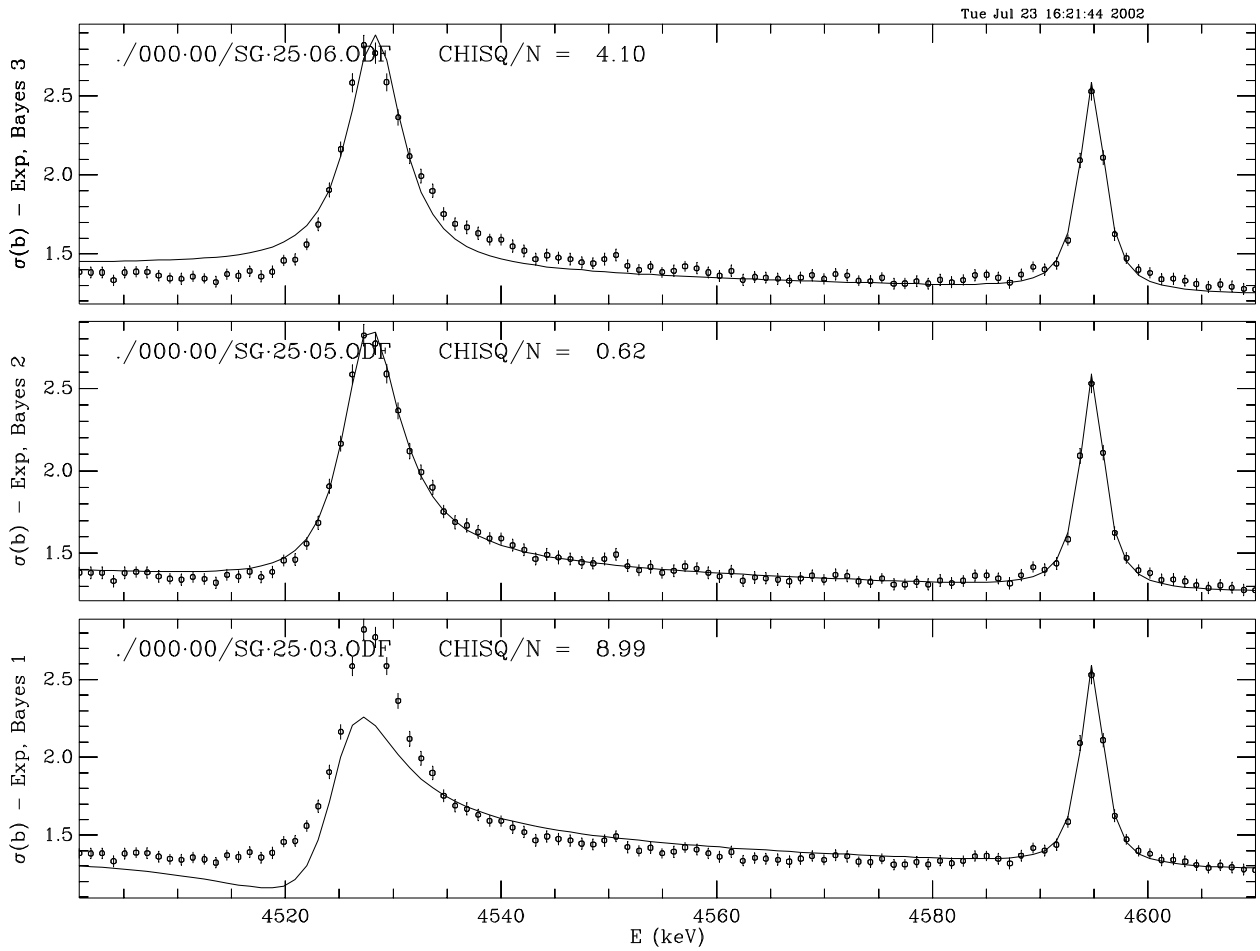


Figure 14: /home/ros/RSAP/EX/12/dosgv25

The file names are written on the "**sgp**" plot as shown in Fig. 14, and fit results are written to files **rsap.chi** and **rsap.sgvout**:

```
RSAP SGV : Here is file rsap.chi

   Resonance 25
 ------------------------------
 Resonance Group    CHISQ/NDAT      Eres(eV)    Ggamma   Gneutron
       25     3         8.9857  4524740.526 2.5000E+02 6.3516E+06 8.8506E+05
       25     5         0.6202  4527389.229 2.5000E+02 4.9415E+06 1.1957E+06
       25     6         4.1012  4528243.660 2.5000E+02 4.6382E+06 1.1648E+06

RSAP SGV : Here is file rsap.sgvout:

   Eres(eV)     Ggamma   Gneutron     Gfiss1     Gfiss2
4524740.526 2.5000E+02 6.3516E+06 8.8506E+05           1 0 1 1   3   200.00
4527389.229 2.5000E+02 4.9415E+06 1.1957E+06           1 0 1 1   5   200.00
4528243.660 2.5000E+02 4.6382E+06 1.1648E+06           1 0 1 1   6   200.00
```

An alternate way of indicating sequential spin groups is illustrated by the command

```
sgr 25, -3, -7
```

This command tells RSAP to do SAMMY fits for spin groups 3 through 7 for resonance 25. The RSAP input file `/home/ros/RSAP/EX/12/dosgv25_3thru7` was used to produce the output shown in Fig. 15. Although 5 SAMMY fits were performed, RSAP plots the best three fits by default. The number of fits plotted may be altered with the **sgb** command.

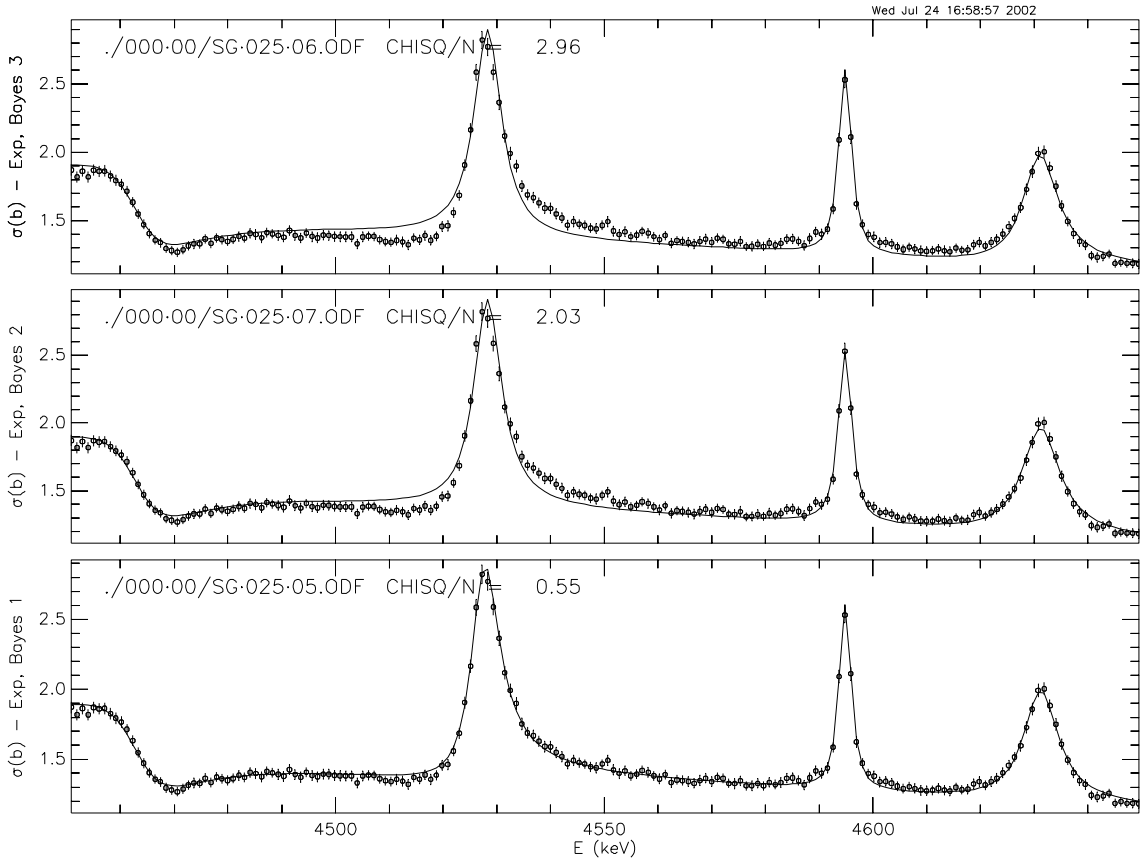


Figure 15: /home/ros/RSAP/EX/12/dosgv25_3thru7

Resonance	Group	CHISQ/NDAT	Eres(eV)	Ggamma	Gneutron	
25	3	5.4591	4524764.278	2.5000E+02	5.9355E+06	7.4464E+05
25	4	11.9090	4525554.599	2.5000E+02	5.4117E+06	4.7090E+05
25	5	0.5497	4527397.612	2.5000E+02	4.9908E+06	1.1212E+06
25	6	2.9556	4528284.932	2.5000E+02	4.7568E+06	1.1009E+06
25	7	2.0291	4528261.389	2.5000E+02	3.6589E+06	2.2829E+06

Eres(eV)	Ggamma	Gneutron	Gfiss1	Gfiss2					
4524764.278	2.5000E+02	5.9355E+06	7.4464E+05		1	0	1	1	3	200.00
4525554.599	2.5000E+02	5.4117E+06	4.7090E+05		1	0	1	1	4	200.00
4527397.612	2.5000E+02	4.9908E+06	1.1212E+06		1	0	1	1	5	200.00
4528284.932	2.5000E+02	4.7568E+06	1.1009E+06		1	0	1	1	6	200.00
4528261.389	2.5000E+02	3.6589E+06	2.2829E+06		1	0	1	1	7	200.00

7.1 Resonances treated sequentially.

Several resonances may be treated sequentially in one RSAP input file. An example RSAP input file for 2 sequential resonances is:

```
    /home/ros/RSAP/EX/12/dosgv_25then27

par /home/ros/RSAP/EX/12/o16/FINAL326.par
sgi /home/ros/RSAP/EX/12/o16/cjav3ndsh_M5.in
sgd /home/ros/NUCDATA/sammy/o16/DATA/cj20742avg3normdsh.dat
###                  1st resonance #, spin group numbers
sgr  25, 4, 5, 6
###  esglo,    esghi
sgv  4500000., 4610000.
###                          automatic plot:
sgp
###                          save ps file for 1st resonance
sys mv sgv1.ps sgv25.ps
###                  2nd resonance #, spin group numbers
sgr  27, 6, 7, 8, 9
sgv  4600000., 4660000.
sgp
###                          save ps file for 2nd resonance
sys mv sgv1.ps sgv27.ps
q
```

Fit results for the 2^{nd} and subsequent resonances are appended to **rsap.chi** and **rsap.sgvout**. The above example file produces a total of 7 SAMMY runs, 3 for resonance 25 and 4 for resonance 27. Note also that a different energy range is used for each resonance.

7.2 Two Resonances treated simultaneously.

Two resonances may be treated simultaneously in one RSAP input file. In this mode RSAP does nested loops over spin groups:

```
do j2=1,j2max     ! spin group loop for resonance 2
        do j1=1,j1max   ! spin group loop for resonance 1

          Edit PAR file and run SAMMY

        enddo
enddo
```

By specifying the maximum of 8 spin groups for each resonance, 64 SAMMY runs could be performed.

An example RSAP input file for "simultaneous" resonances is:

```
    /home/ros/RSAP/EX/12/dosgv25and26

###       Vary spin groups for both res. 25 and res. 26
par /home/ros/RSAP/EX/12/o16/FINAL326.par
sgi /home/ros/RSAP/EX/12/o16/cjav3ndsh_M5.in
sgd /home/ros/NUCDATA/sammy/o16/DATA/cj20742avg3normdsh.dat
###  resonance number, spin group numbers
sgr  25, 4, 5, 6, 7, 10
sgr  26, 8, 9
###  esglo,    esghi
sgv  4500000., 4610000.
sgp
```

For this example, ODF and final PAR files for each spin group fit are saved in the subdirectories **026_08** and **026_09**. The saved files are:

```
./026_08/SG_025_04.PAR        ./026_08/SG_025_04.ODF
./026_08/SG_025_05.PAR        ./026_08/SG_025_05.ODF
./026_08/SG_025_06.PAR        ./026_08/SG_025_06.ODF
./026_08/SG_025_07.PAR        ./026_08/SG_025_07.ODF
./026_08/SG_025_10.PAR        ./026_08/SG_025_10.ODF

./026_09/SG_025_04.PAR        ./026_09/SG_025_04.ODF
./026_09/SG_025_05.PAR        ./026_09/SG_025_05.ODF
./026_09/SG_025_06.PAR        ./026_09/SG_025_06.ODF
./026_09/SG_025_07.PAR        ./026_09/SG_025_07.ODF
./026_09/SG_025_10.PAR        ./026_09/SG_025_10.ODF
```

The file names are written on the "**sgp**" plot as shown in Fig. 16. The upper plot shows the three best fits for resonance 26, spin group 8, and the lower plot shows the three best fits for resonance 26, spin group 9. Fit results are written to files **rsap.chi** and **rsap.sgvout**:

```
RSAP SGV : Here is file rsap.chi

   Resonance 25
   Resonance 26
---------------    ---------------    ----------   ----------     ------   --------
Resonance Group    Resonance Group    CHISQ/NDAT     Eres(eV)     Ggamma   Gneutron
       26
              8          25     4        17.8380  4525472.200 2.5000E+02 4.8743E+06 5.7239E+04
              8          25     5         0.6202  4527389.229 2.5000E+02 4.9415E+06 1.1957E+06
              8          25     6         4.1012  4528243.660 2.5000E+02 4.6382E+06 1.1648E+06
              8          25     7         3.0712  4528323.287 2.5000E+02 3.5306E+06 2.2838E+06
              8          25    10         6.0854  4527360.848 2.5000E+02 2.7106E+06 3.1953E+06

              9          25     4        19.2822  4525403.442 2.5000E+02 4.7154E+06 5.6229E+05
              9          25     5         0.6204  4527412.089 2.5000E+02 4.9870E+06 1.2924E+06
              9          25     6         4.0904  4528266.812 2.5000E+02 4.6799E+06 1.2451E+06
              9          25     7         3.0909  4528318.713 2.5000E+02 3.5743E+06 2.3120E+06
              9          25    10         6.1926  4527358.600 2.5000E+02 2.7273E+06 3.1474E+06
```

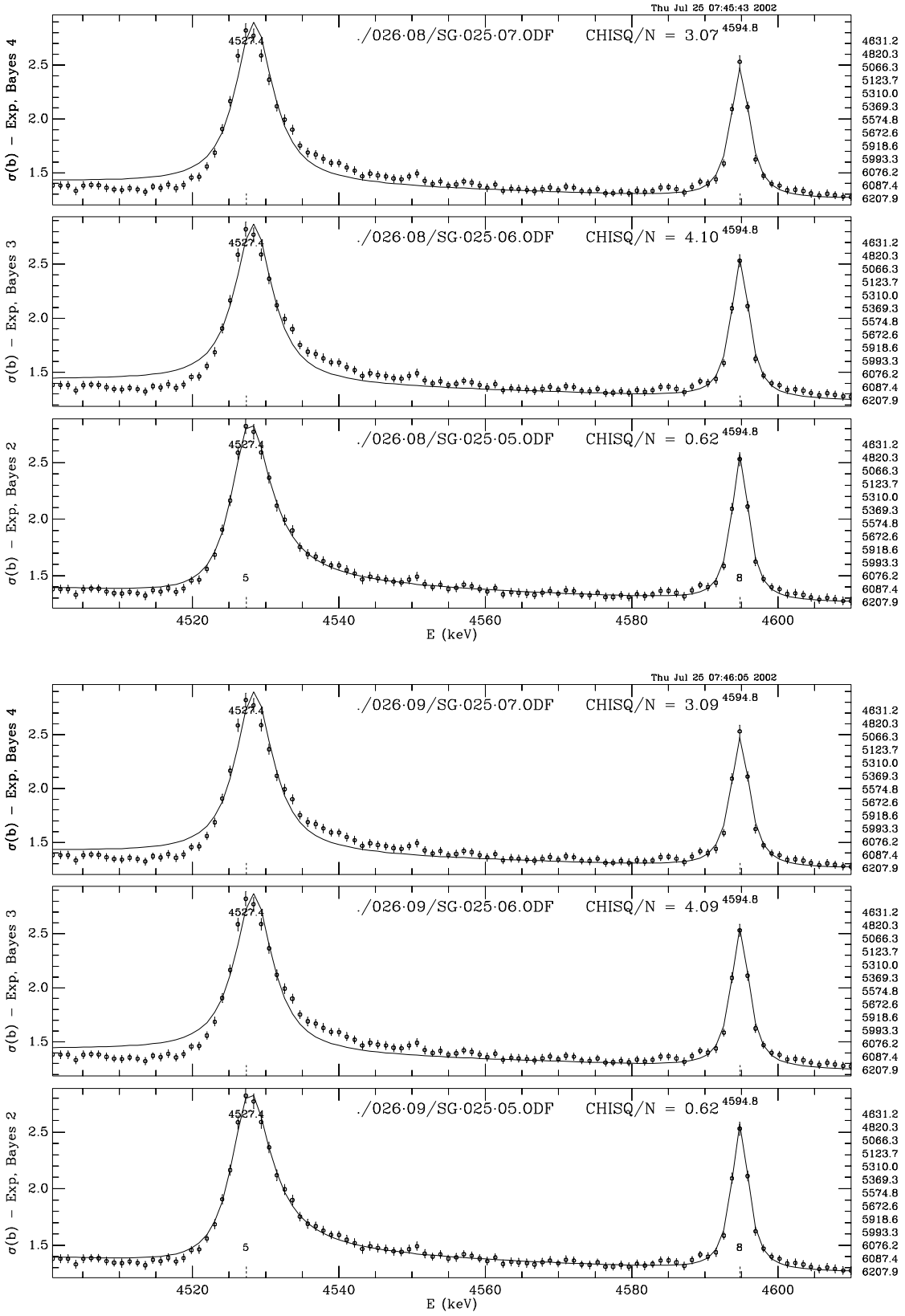


Figure 16: /home/ros/RSAP/EX/12/dosgv25and26. Upper plot: 3 best fits for resonance 26, spin group 8. Lower plot: 3 best fits for resonance 26, spin group 9.

8 Visual Uncertainty Analysis

Treatment of uncertainties in analysis of neutron cross section data with SAMMY is discussed in some detail by N. M. Larson [2] and others (see, for example, D. C. Larson, et al.[6]). Unfortunately, for many data sets, errors are not reported in sufficient detail to permit a rigorous analysis, particularly the uncertainties associated with calibrations, background subtractions, etc. This can lead to evaluations with resonance parameter covariances that are too small or too large. Two graphical analysis procedures have been implemented in RSAP to aid the user in determination of uncertainties in resonance widths. Each procedure consists of generating a series of SAMMY calculations for different width values of specified resonances followed by overlay and/or stacking of plots.

8.1 UNC procedure

The **UNC** procedure consists of a simple RSAP input file specifying SAMMY input and PAR files, one or more resonances, an energy range for the calculation, and up to 8 width values. For each specified resonance and each specified width, RSAP automatically edits the PAR file, runs SAMMY, and plots the results. The specifiers and their arguments are :

```
par SAMMY_PAR_file_name
sgi SAMMY_input_file_name
sgd SAMMY_data_file_name
unr resonance_number1, resonance_number2, ...
unw width_scale1, width_scale2, ...
unt itype
unc eulo, euhi
```

The `par`, `sgi`, `sgd`, and `unr` specifiers are required. The `resonance_number` corresponds to the record number in the PAR file. The arguments of `unw` are width scale factors in percent. The type of width (CAPTURE, NEUTRON, FISSION1, FISSION2) is given by `unt`. The default type is NEUTRON. The action specifier **unc** tells RSAP to do a "no Bayes" SAMMY calculation over the energy range (eV) from **eulo** to **euhi** for each width scale factor. For a given calculation, the width scale factor is applied to all resonances enumerated in `unr`. An example file is reproduced below.

`/home/ros/RSAP/EX/22/inunc`

```
par /home/ros/RSAP/EX/12/o16/FINAL326.par
###                                SAMMY input file
sgi /home/ros/RSAP/EX/21/cjav3ndsh_nob.inp
###                                SAMMY data file
sgd /home/ros/RSAP/EX/12/o16/cj20742avg3normdsh.dat
###      resonance numbers
unr  25, 26
###      width scale factors in percent
unw  90, 100, 110
###                         energy range (eV) for calculation
unc  4500000., 4610000.
```

No parameters are varied in the SAMMY calculations. RSAP does not modify the original PAR and INP files.

PLT and LPT files for each width scale factor calculation are saved in the user's current directory. For the above example, the saved files are:

```
UNC_NEUT_090.PLT        UNC_NEUT_090.LPT
UNC_NEUT_100.PLT        UNC_NEUT_100.LPT
UNC_NEUT_110.PLT        UNC_NEUT_110.LPT
```

File names and values of the customary χ^2/N are written on the stacked plot as shown in Fig. 17.

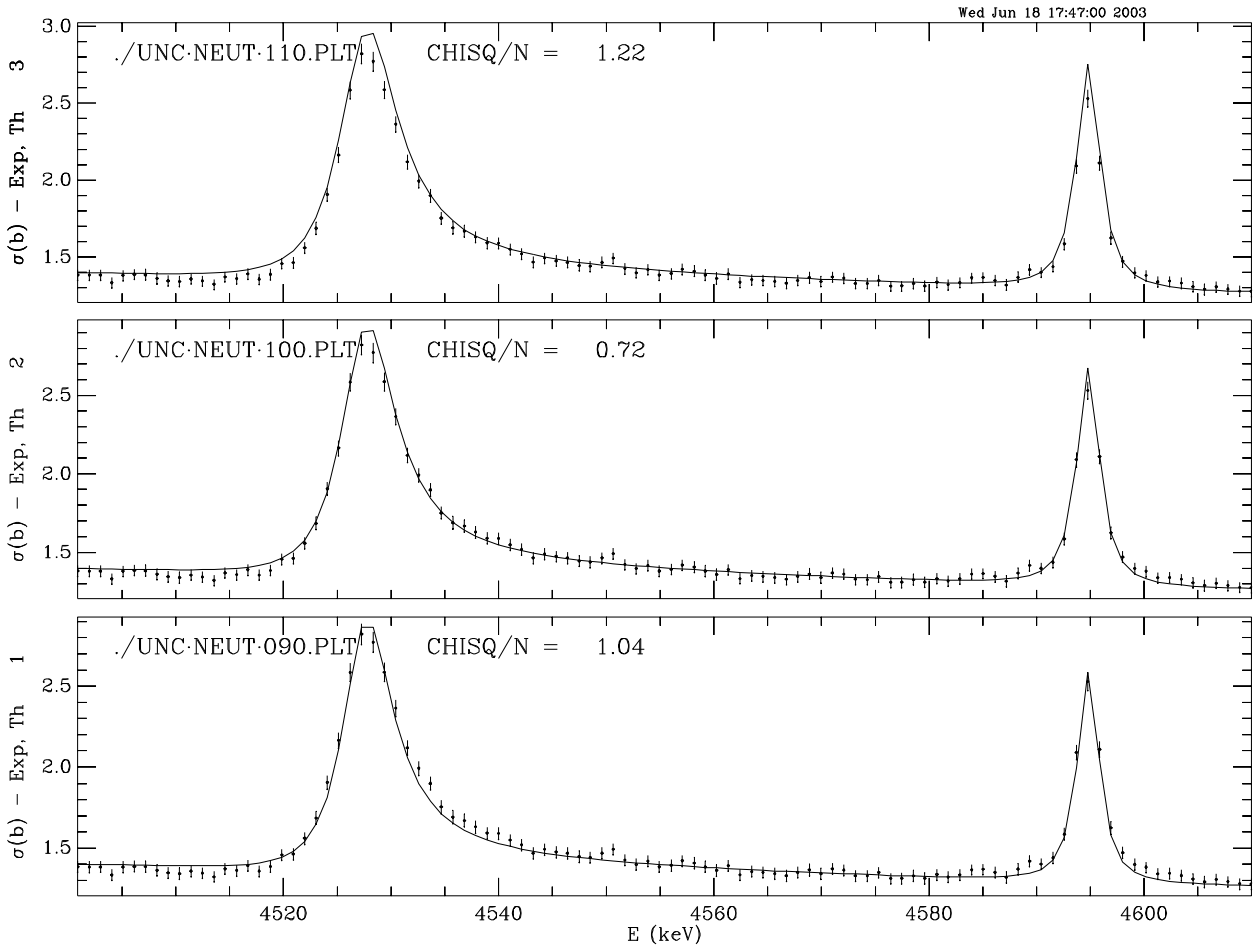


Figure 17: /home/ros/RSAP/EX/22/inunc. Sample plot for UNC procedure.

8.2 UNA - automated, interactive uncertainty procedure.

A "PUBLISH" statement in the inp file will direct SAMMY to produce a tab-delimited file, `SAMMY.PUB`, that contains uncertainties for all flagged resonance parameters. The **UNA** procedure allows one to perform and view "no Bayes" calculations for selected resonances with width values corresponding to the PAR file width G, and widths G ± U, where U is the uncertainty in G read from `SAMMY.PUB`. The U values can be scaled by a specified factor. In the process RSAP will create a new file, `rsap.PUB`, which is identical to `SAMMY.PUB` except that the specified U values are replaced by the scaled U values. The user may select the type of width (capture, neutron, fission) to vary. By default, stacked and overlaid screen plots of the three calculations are produced. Specific resonances or a range of resonances (maximum 512) may be selected with the `unr` specifier.

An example RSAP input file is shown below:

```
/home/ros/RSAP/EX/21/inuna

    ###             SAMMY.PUB must be in the user's current directory
    cp /home/ros/RSAP/EX/21/SAMMY.PUB SAMMY.PUB
    ###                                          PAR file - for widths
    par /home/ros/RSAP/EX/12/o16/FINAL326.par
    ###                                          SAMMY input file
    sgi /home/ros/RSAP/EX/21/cjav3ndsh_nob.inp
    ###                                          SAMMY data file
    sgd /home/ros/RSAP/EX/12/o16/cj20742avg3normdsh.dat
    ###           resonance numbers
    unr  25, 26, 27
    ###
    ###     itype =  1,2,3,4 says CAPTURE,NEUTRON,FISSION1,FISSION2 widths
    unt 2
    ###               unp iview, iprint
    ###  iview  0,1,2,3 for no  screen plot, stack, overlay, both.   Default 3.
    ###  iprint 0,1,2,3 for no printer plot, stack, overlay, both.   Default 0.
    ###
    unp  3
    ###           scale SAMMY.PUB uncertainties by factor of 3.0 and do calculations
    ###           calculation range:  Eres - 5.*Gtotal < E < Eres + 5.*Gtotal
    una  3.0, 5.0
```

The first argument of `una` is the scale factor for U, and the second argument is half the number of total widths in the calculation range (default 5.0). Three "no Bayes" SAMMY calculations are done for the first resonance (25) and plotted. Then RSAP prompts the user for a new scale factor. If a new scale factor is entered, RSAP repeats the three calculations and plots. This loop continues until no value ("RETURN") is entered; then RSAP proceeds to do calculations for the next resonance (26). After each new scale factor is entered, RSAP updates the output uncertainty file `rsap.PUB`.

For this example, PLT and LPT files for each width value calculation are saved in the subdirectories **025**, **026**, and **027**. File names indicate the scale factors; for example, `300M` corresponds to a calculation with width G - 3.00*U, and `300P` corresponds to a calculation with width G + 3.00*U. Also the file names indicate the type of width: NEUT, CAPT, FIS1, or FIS2. For the example

above, the saved files are:

```
./025/UNC_NEUT_PUB_300M.PLT        ./025/UNC_NEUT_PUB_300M.LPT
./025/UNC_NEUT_PUB_000.PLT         ./025/UNC_NEUT_PUB_000.LPT
./025/UNC_NEUT_PUB_300P.PLT        ./025/UNC_NEUT_PUB_300P.LPT

./026/UNC_NEUT_PUB_300M.PLT        ./026/UNC_NEUT_PUB_300M.LPT
./026/UNC_NEUT_PUB_000.PLT         ./026/UNC_NEUT_PUB_000.LPT
./026/UNC_NEUT_PUB_300P.PLT        ./026/UNC_NEUT_PUB_300P.LPT

./027/UNC_NEUT_PUB_300M.PLT        ./027/UNC_NEUT_PUB_300M.LPT
./027/UNC_NEUT_PUB_000.PLT         ./027/UNC_NEUT_PUB_000.LPT
./027/UNC_NEUT_PUB_300P.PLT        ./027/UNC_NEUT_PUB_300P.LPT
```

RSAP command files `cmf025`, `cmf026`, and `cmf027` are saved in the user's current directory so that plots for resonance 25, for example, can be viewed later by typing"`cmf cmf025`" at the RSAP prompt. Plots for all resonances may be viewed with"`rsap < rsap.unacmf`".

Note that the width values are read from the specified PAR file, **not** from SAMMY.PUB.

For this example, both the stacked and overlaid plots for resonance 25 are shown in Fig. 18. For resonances 26 and 27 the overlaid plots are presented in Fig. 19.

Up to 512 resonances may be treated sequentially by entering negative resonance numbers; for example, the command

```
unr -185, -264
```

would specify all resonances from 185 to 264.

The user may "automate" the UNA procedure by turning off screen plots with the command

```
unp 0
```

Then RSAP will cycle through the sequence of specified resonances, applying the specified scale factor to the SAMMY.PUB uncertainties, doing three calculations for each resonance, and updating rsap.PUB. The user will not be prompted for additional input. After the last resonance is done, the user may view calculations for particular resonances with the RSAP command files"`cmfnnn`", where `nnn` is the resonance number. Plots for all resonances may be viewed with "`rsap < rsap.unacmf`".

Due to the interactive feature of the UNA procedure, the user must start it at the RSAP prompt:

```
RSAP6> cmf myfile
```

where `myfile` is the user file containing the UNA commands (`par, sgi, sgd, unr,` etc.). The directive `rsap < myfile` will **not** work.

RSAP writes an output file, `rsap.unaout`, containing widths and uncertainties expressed in percent as shown in the example below.

```
UNA:  Widths from file /home/ros/RSAP/EX/12/o16/FINAL326.par
UNA:  Uncertainties from SAMMY.PUB

UNA:                        ---------- Widths --------     ------ Uncertainties ----
 Res    Energy    GammaTOTAL   CAPT   NEUT   FIS1   FIS2     CAPT   NEUT   FIS1   FIS2
        (eV)         (eV)       %      %      %      %        %      %      %      %
  25 4527358.5     5852.600  0.004 85.289 14.707  0.000     0.00   1.82  11.49   0.00
  26 4594830.6     1828.090  0.014 76.151 23.836  0.000     0.00   2.86  13.22   0.00
  27 4631214.8     7079.750  0.004 45.240 54.756  0.000     0.00   2.60   5.98   0.00
```

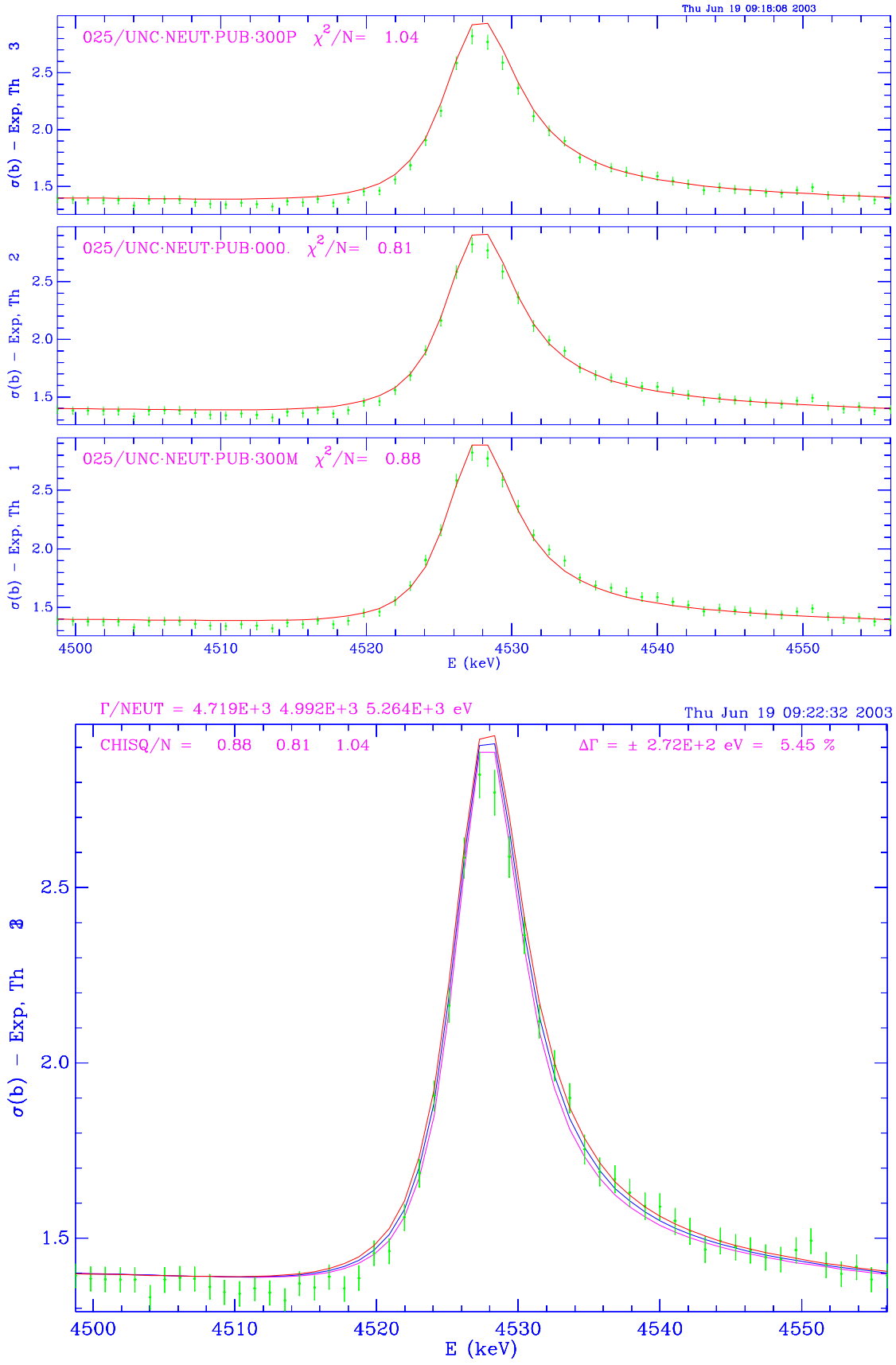


Figure 18: /home/ros/RSAP/EX/21/inuna. Upper plot: 3 SAMMY "no Bayes" calculations for resonance 25, stacked. Lower plot: 3 calculations for resonance 25, overlaid.

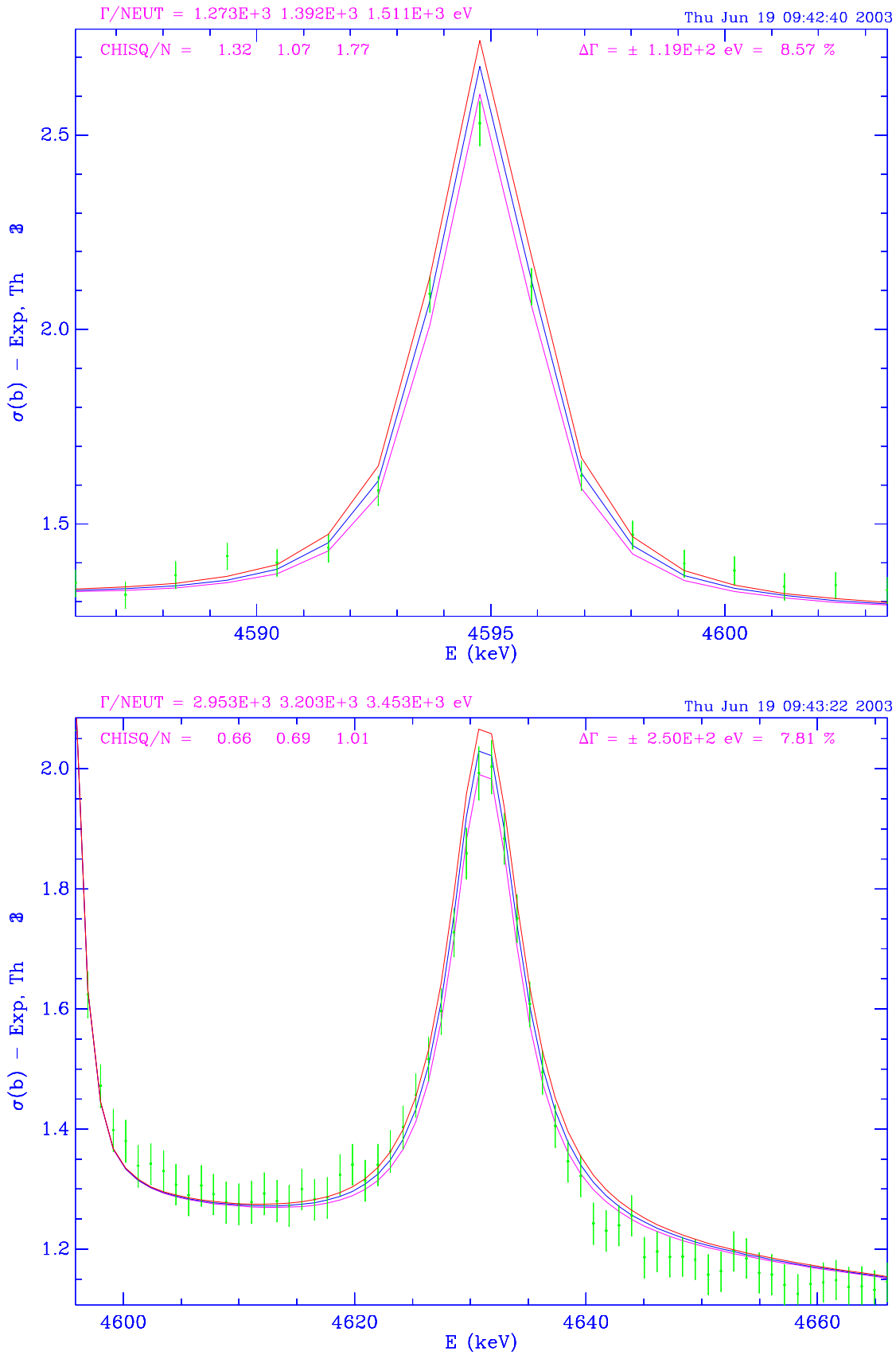


Figure 19: /home/ros/RSAP/EX/21/inuna. Upper plot: overlay of 3 SAMMY "no Bayes" calculations for resonance 26. Lower plot: overlay of 3 calculations for resonance 27.

Acknowledgements

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References

[1] R. O. Sayer, *RSAP - A Code for Display of Neutron Cross Section Data and SAMMY Fit Results*, Oak Ridge National Laboratory Report ORNL/TM-2000/15 (2000).

[2] N. M. Larson, *Updated Users' Guide for Multilevel R-Matrix Fits to Neutron Cross Section Data Using Bayes' Equations*, Oak Ridge National Laboratory Report ORNL/TM-9179/R6, (2003).

[3] R. E. MacFarlane and D. W. Muir, *The NJOY Nuclear Data Processing System Version 91*, Los Alamos National Laboratory Report LA-12740-M (1994) .

[4] M. J. LeBrun, G. Furnish, and T. Richardson, The PLPLOT Plotting Library (1994). http://sourceforge.net/projects/plplot

[5] M. A. Mariscotti, Nucl. Inst. Methods **50**, 309 (1967).

[6] D. C. Larson, N. M. Larson, and J. A. Harvey, *ORELA Flight Path 1: Determinations of Its Effective Length vs Energy, Experimental Energies, and Energy Resolution Function and Their Uncertainties*, Oak Ridge National Laboratory Report ORNL/TM-8880 (1984).

APPENDICES

A. Example Script for SAMMY + RSAP Run

```
set sammy=/home/nml/m6/exe/sammy
set rsap=/home/ros/RSAP/v6/gorsap6
#
#########                    make rsap input file for device x
cat <<eod> inx
par JohnFowl235_990203.par
odf SAMMY.ODF
tit JohnFowl235_990203 3.784              Title (a32)
ops  1 100 1 1 1
x
1 deb 2200.,2500.,0.0,1.00        (a2, a4, 4f10)
q
eod
##########                     make SAMMY input file
cat <<eod> input
/home/ros/NUCDATA/sammy/o16/990203/JohnFowl235.in
/home/ros/NUCDATA/sammy/o16/990203/JohnFowl235_990203.par
/home/ros/NUCDATA/sammy/o16/DATA/JohnFowl235_HC981111.dat 2285000.0,2490000.
eod
$sammy < input > output
#
$rsap < inx
```

B. Example rsap.ratexpth File

```
 E(keV) SigmaExp(b) Error(b)  Theory(b)   BAYES(b)  100*  100*
                           (Th/Exp-1) (BAYES/Exp-1)
200.8193 3.4680E+00 0.02500 3.50496E+00 3.50464E+00 1.066 1.056
201.8257 3.4620E+00 0.02570 3.50363E+00 3.50331E+00 1.203 1.193
202.8397 3.4020E+00 0.02570 3.50231E+00 3.50198E+00 2.949 2.939
203.8613 3.4740E+00 0.02550 3.50099E+00 3.50066E+00 0.777 0.768
204.8908 3.4410E+00 0.02500 3.49968E+00 3.49935E+00 1.705 1.696
205.9279 3.4510E+00 0.02440 3.49837E+00 3.49804E+00 1.373 1.363
.............................................................
6200.874 9.6110E-01 0.13790 9.40398E-01 9.41881E-01 -2.154 -2.000
6211.689 1.0610E+00 0.13970 9.32850E-01 9.34306E-01 -12.078 -11.941
6222.533 9.5580E-01 0.13670 9.25973E-01 9.27403E-01 -3.121 -2.971
6233.404 9.9550E-01 0.13940 9.19679E-01 9.21084E-01 -7.616 -7.475
```

C. Example rsap.parcom File

```
Wed Jan 27 14:46:35 EST 1999
duanesh_990126.par
Res Grp    E(keV)     E/SAM      GamC1 GamC1/SAM    GamC2  GamC2/SAM  Vary    Eunc.
  1   1 -12024.00 -12021.00    9106.20   9126.20                      1 0 1    10.0
  2   1  -4469.30  -4469.20    5469.30   5485.00                      1 0 1     1.0
  3   3    434.30    434.30      44.17     44.40                      1 0 1     0.2

  4   4   1000.28   1000.25      99.64    100.43                      1 0 1     0.2
  5   3   1309.36   1309.36      43.17     43.35                      1 0 1     0.2
.............................................................
 37   6   6076.13   6076.13       4.76      4.81      2.00      2.00  1 0 1     0.2
 38   2   6087.91   6087.90      14.53     14.57      4.51      4.51  1 0 1     0.2
 39   7   6387.66                 9.91     10.01     35.98     36.01  0 0 0     0.2

 40   3  10980.19  10989.91   14338.00  14369.00                      1 0 1   100.0
 41   2  18777.06  18755.84   27453.00  27495.00                      1 0 1   100.0
 42   4  16158.63  16146.03    1926.00   1930.90                      1 0 1   100.0


RADIUS PARAMETERS FOLLOW
   3.77736   3.7773611-1 1 2 3 4 5 6 7 8 0 1
   6.49920   6.4992011-1 1 2 3 4 5 6 7 8 0 2

NORMAlization and "constant" background follow
 1.0038828 0.000E+00 0.000E+00 0.000E+00 0.000E+00 0.000E+00 1 0 0 0 0 0

COVARIANCE MATRIX IS IN BINARY FORM

  Grp  Res          er         gam       samer      samgam     samgam2
    1    1  -12024.000    9106.200  -12021.000    9126.200       0.000    s1/2
    1    2   -4469.300    5469.300   -4469.200    5485.000       0.000
    1    3    2378.121     160.770    2377.930     160.360       0.000
.............................................................
    7    1    1651.380       4.004    1651.380       4.053       0.000    f7/2
    7    2    3766.949      18.148    3766.947      18.350       0.015
    7    3    5123.835      22.531    5123.806      22.761       2.016
    7    4    6387.658       9.912    6387.658      10.006      36.010

    8    1    4594.304       1.492    4594.304       1.515       0.203    g7/2
    8    2    5918.549      19.342    5918.571      19.624       2.501
  Grp  Res          er         gam       samer      samgam     samgam2
 CUSTOMARY CHI SQUARED DIVIDED BY NDAT =   1.53943
 CUSTOMARY CHI SQUARED DIVIDED BY NDAT =   1.48805
 CUSTOMARY CHI SQUARED DIVIDED BY NDAT =   1.48802
```

D. PLPLOT metafiles and plrender

The discussion herein follows closely the information given in the PLPLOT documentation [3]. A PLPLOT metafile is a binary, device-independent stream of bytes that may be rendered with the PLPLOT utility, **plrender**. To render the metafile, **rsap.meta,** type:

```
plrender [options] rsap.meta
```

where

```
options(partial list):
 -dev name            Output device name
 -o name              Output filename
 -px number           Plots per page in x
 -py number           Plots per page in y
 -geometry geom       Window size, in pixels (e.g. -geometry 400x300)
 -wplt xl,yl,xr,yr    Relative coordinates [0-1] of window into plot
 -mar margin          Margin space - relative coord (0 to 0.5, def 0)
 -a aspect            Page aspect ratio (def: same as output device)
 -jx justx            Page justification in x (-0.5 to 0.5, def 0)
 -jy justy            Page justification in y (-0.5 to 0.5, def 0)
 -ori orient          Plot orientation (0,2=landscape, 1,3=portrait)
 -bg color            Background color (0=black, FFFFFF=white)
```

A complete list of options may be obtained by typing "plrender –h". For example, to make a color postscript file, **rsap_port**, in portrait orientation on a white background:

```
plrender --dev psc --bg FFFFFF --o rsap_port --ori 3 rsap.meta
```

JPEG output (for PLPLOT version 5.1.0 and later) may be produced:

```
plrender --dev jpg --bg FFFFFF --o rsap.jpg rsap.meta
```

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