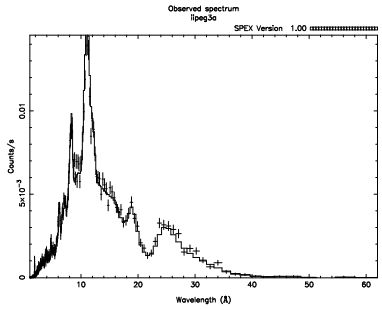
SRON – SPEX

SPEX User's/Tutorial Manual

SRON/SPEX/TRUM

SPEX Version 1.06

April 25, 1995



prepared by

J.S. Kaastra	SRON Utrecht
R. Mewe	SRON Utrecht
H. Nieuwenhuijzen	RUU, SRON Utrecht
F. van der Wolf	SRON Utrecht

Preface

This is the user's manual of SPEX, version 1.06, released 25 april, 1995. A novice user is advised to read at least Chapter 2, which gives an example of a typical SPEX-session.

Contents

Chapter 1

Introduction

1.1 What is SPEX?

The advent of a new series of X-ray satellites with high sensitivity and spectral resolution such as *EUVE*, *ASCA*, *SAX*, *AXAF*, and *XMM* strongly demands the availability of spectral codes with higher accuracy and more detail than has been available. The menu-driven **SPE**ctral **X** & UV analysis software package **SPEX** has been developed at the Space Research Organization Netherlands (**SRON**) for complex modeling of hot astrophysical plasmas in view of fitting space-based observations. It has been applied in analyzing archival *EXOSAT* and *EINSTEIN* data, recent *EUVE* & *ASCA* data, and in simulating *AXAF* & *XMM* spectra. SPEX encompasses a number of sophisticated modules for the computation of the physical parameters and associated emergent spectra of a variety of plasmas including optically thin plasmas - such as stellar coronae and supernova remnants, photo-ionized plasmas, and optically thick plasmas. The model spectra can be convolved with instrumental response functions and compared with observations. Examples of various spectral simulations are shown. In short, SPEX offers advantages such as:

- advanced graphical and ascii-file display of plasma- and spectral parameters
- extended energy range from UV to X-rays
- combination of many different models
- response matrices for various instruments like EUVE, SAX, ASCA, XMM & AXAF
- independent choice of energy grid and rebinning (important for XMM & AXAF)
- combination of observations from different instruments for simulation & fitting
- differential emission measure (DEM) analysis and other fitting methods
- complicated plasma models such as supernova-remnant and coronal-loop models
- non-equilibrium ionization and photo-ionization
- extended documentation on software and physical background

Some details of performance are discussed below.

1. **Modeling**
   (a) Complete restructuring of the plasma part of our code and calculation of complex models such as supernova remnants (SNRs) (multilayer non-equilibrium ionization), stellar coronae (DEM analysis), photo-ionized plasmas, etc. as compared to only equilibrium plasmas in the code implemented late 1992 in XSPEC (version 8.23) under the name MEKA.

2. **Display**
   (a) In addition to the display, output or plot of the total spectrum, we are also interested in some other properties: radial brightness profile, ion concentrations, line identifications, hydrodynamical properties, plasma rates etc.
3. **Response matrices**
   (a) If the response matrix for a given instrument has insufficient energy resolution to disentangle line features, it is necessary to choose another energy grid, and to rebin the response matrix to the chosen grid (important e.g., for AXAF and XMM).
   (b) More freedom in combining observations from different instruments (e.g., adding spectra channel by channel) and rebinning the data.
4. **Fitting**
   (a) CPU intensive models, like those for supernova remnants, require a lot of model evaluations for one iteration step if the classical Levenberg-Marquardt method is applied, at least where many abundances have to be determined simultaneously. We have reduced the number of model evaluations by making use of the principle that the spectrum is linear in the elemental abundances, hence given the other model parameters, the abundances can be determined using a simple matrix inversion. This increases the fitting speed considerably.
   (b) Differential emission measure (DEM) analysis is possible in SPEX; it uses a completely different way of solution from the classical Levenberg-Marquardt method otherwise used in spectral fitting.

In addition, some general requirements such as modularity, compact documentation, transportability, adaptability to various instruments, and flexibility to include more or new atomic data have led us also to the restructuring of our software.

1.2 Development of Spectral Codes at SRON

1. Mewe (1972, Paper I; 1975, Paper II): first approach to optically thin model
   (a) calculations of Collision Ionization Equilibrium (CIE) model
2. Mewe & Gronenschild (1978, Paper III; 1981, Paper IV):
   (a) basic papers on continuum & line emission with full description of parameters
3. Mewe, J. Schrijver & Gronenschild (1974-1980): first non-equilibrium calculations
   (a) development Non-Equilibrium Ionization (NEI) model for solar flares (1974)
   (b) first application of NEI Sedov model to supernova remnants (1979)
4. Mewe, J. Schrijver (1974-80): extended calculations on He-like ions
5. Sylwester, J. Schrijver & Mewe: development of iterative DEM code (1979)
6. Mewe, Gronenschild & van den Oord (1985, Paper V), Mewe, Lemen & van den Oord (1986, Paper VI):

(a) extended line & continuum emission CIE 1985 codes with full description

7. Kaastra, Jansen (1984-93):
   (a) EXOFIT-code for spectral fitting of EXOSAT data
   (b) enhanced speed of ion balance calculations by a matrix inversion (instead of 4th-order Runge-Kutta)
   (c) development of various NEI supernova remnant models
8. Kaastra and Mewe (1992-93):
   (a) update & extension of continuum & line emission
   (b) development of new DEM code (with C.J. Schrijver, Alkemade, van den Oord)
   (c) development of photo-ionization model & calc. of Auger ionization
   (d) installment of MEKA code at HEASARC/NASA (1992)
9. Kaastra, Mewe (1992–), development of SPEX code:
   (a) structuring the code (with Nieuwenhuijzen)
   (b) model development & implementation
   (c) updating atomic physics and databases including:
   - improved Fe L-shell (Fe XXIV–XVII) calculations (with Liedahl, HULLAC code at Livermore)
   - Arnaud-Raymond (1992) ionization balance
   - addition of about 60 DR lines to the He-like Mg lines at 1.3 keV
   - addition of over 300 EUV lines from Landini, Monsignori Fossi (1990) with corrections
   - improved calculations of Fe XVI–VIII

   (d) documentation of the code (with Nieuwenhuijzen) and of the physics
   (e) installment of SPEX at HEASARC/NASA and availability to the community (1995) (to be agreed)

1.3 Spectral components available in SPEX

1. **CIE model**: Optically thin, steady-state plasma in Collisional Ionization Equilibrium. Ionization & excitation occur by electron impact. Ionization is balanced by radiative & dielectronic recombination.
2. **NEI model**: Discontinuous temperature jump causing Non-Equilibrium Ionization (transient optically thin plasmas like SNR and stellar flare). Heating process yields temperature rise so fast that the ionization cannot follow this so that ionization balance is far out of equilibrium.
3. **SNR models**: SuperNova Remnant (optically thin, multi-temp. structure, transient state). Prototype of a strongly NEI plasma. We distinguish between the following models:
   (a) Sedov (1959) (adiabatic) model
   (b) Chevalier (1982) (adiabatic plus reverse shock) model

(c) Hamilton (1985) (adiabatic plus reverse shock, clumps) model

(d) Solinger et al. (1975) (isothermal) model

(e) Band (1988) (isothermal or isentropic plus reverse shock) model.

4. **DEM model**: differential emission measure (DEM) distribution of a multi-temperature, optically thin plasma such as a stellar corona or a cluster of galaxies in a steady-state.

   In addition the following simple models are available:

5. **Delta function**: infinitely narrow spectral line.
6. **Gaussian line**: single spectral line broadened by e.g. thermal Doppler, instrumental, or turbulent velocity effects.
7. **Power Law $E^{-\alpha}$ (nonthermal) spectrum**, e.g. AGN, stellar flare.
8. **Black-Body spectrum** (optically thick, single temperature)
9. **Modified Black-Body spectrum**: modified by Compton scattering on nonrelativistic electrons (optically thick, single temperature, e.g. active galactic nucleus (AGN)).

   Further, SPEX encompasses the following multiplicative components that can be applied in arbitrary sequence to any combination of additive components:

10. **Redshift**: cosmological redshift.
11. **Absorption**: X-ray absorption from the diffuse ISM according to Morrison & McCammon (1983).
12. **Absorption**: EUV absorption from the diffuse ISM according to Rumph et al. (1994).
13. **Absorption**: continuum absorption by a hot plasma in collisional ionization equilibrium (CIE).

1.4 SPEX Models under development

The following more sophisticated models are currently under development:

1. **Active-Region-Loop model**: Optically thin, multi-temperature, stationary plasma in coronal loop structures (G.H.J. van den Oord).
2. **LTE atmosphere model**: Optically thick atmosphere with temperature stratification, in Local Thermal Equilibrium, with irradiation by an external radiation field, e.g., a white dwarf, the stellar wind of an O star) (J. Heise).
3. **Photo-ionized model**: Nebular-type plasma with ionization dominated by external radiation field (e.g., X-ray binaries, AGNs). The ionization balance is set up between photo-ionization and radiative recombination (J.S. Kaastra).

1.5 SPEX Document structure

The SPEX documentation is available in two levels: a **user level** and a **program level** . The user level (see Fig. 1.1) provides all the information needed to install and run the SPEX program and includes a description of the physical background associated with the software package. It also provides information about the instrumental response of several X–ray observing satellite instruments and a cookbook with tips and tricks for experienced users.

The program level (see Fig. 1.2) contains information about the software architecture and detailed descriptions of subroutines used by the SPEX program. It also explains how to install SPEX on your own system and what soft- and hardware requirements are to be met.

A novice user is advised to read this manual and the physical background. A sample session in chapter 3 shows the scope of the SPEX environment. Experienced users are encouraged to go through the other manuals and send suggestions of improvement to the addresses listed below.

1.6 Acknowledgements

We would like to express our special thanks to numerous people who have substantially contributed to the development of the work on X-ray spectral modelling, in chronological order: J.Schrijver, E.H.B.M. Gronenschild, J. Sylwester, A. Fludra, G.H.J. van den Oord, J.R. Lemen, F.A. Jansen, R.J.C. Smeets, C.J. Schrijver, F.J.M. Alkemade, C.J.Th. Gunsing, D. Verner, J. Stil, I. Eggenkamp, E. Philippus, and G.-J. Bartelds.

During the years the many people have contributed as follows:

The philosophy of the fitting procedure is based on the experiences obtained with the fitting of EXOSAT data, especially on the software package ERRFIT designed by Jansen and Kaastra. The non-equilibrium ionization balance routine was developed by Jansen, based on earlier work by J. Schrijver (1974) and Gronenschild (1981). The SNR models are based on the work by Kaastra and Jansen (1992). The Hamilton SNR model is programmed by Stil. The line and continuum emission routines were written by Kaastra, based on previous routines by Mewe, Gronenschild, van den Oord, and Lemen (1981-1986). Lemen, Smeets, and Alkemade developed an earlier version (1986-1990) of a spectrum synthesis program. The original DEM modelling was based on the work by Sylwester and Fludra (1980), while the current DEM algorithm has been designed by C.J. Schrijver and Alkemade. The line and continuum emission data are completely based on the work by Mewe and Kaastra. The photo-ionization cross-sections have been calculated by Verner and implemented by Kaastra. The complete menu structure is written by Kaastra with advice from Nieuwenhuijzen, while Philippus helped to design the windows version. Nieuwenhuijzen contributed to the software design and Kaastra was responsible for the whole software implementation. Eggenkamp, Alkemade, Stil, Bartelds and van der Wolf helped in testing the software and contributed many new ideas. The documentation has been prepared – with starting help by Gunsing – by van der Wolf and Nieuwenhuijzen (for the manual structure and introduction), by Mewe (for the scientific background), by Kaastra (for the software description), and by Mewe and Kaastra together for the description of models and instrument response functions.

The project supervision is in the hands of Mewe, Kaastra and Nieuwenhuijzen.

User level

- **User's/Tutorial Manual: SRON/SPEX/TRUM**
- **Physical Background:**
  - **SRON/SPEX/TRPB01:** *X-Ray spectroscopy*
  - **SRON/SPEX/TRPB02:** *Ionization and energy balance in collisionally and photo-ionized plasmas*
  - **SRON/SPEX/TRPB03:** *Continuum radiation processes*
  - **SRON/SPEX/TRPB04:** *Line excitation processes*

    With appendices:
    - **SRON/SPEX/TRPB04a:** *List of input line paramters*
    - **SRON/SPEX/TRPB04b:** *Atlas of dielectronic recombination lines*
    - **SRON/SPEX/TRPB04c:** *Atlas of innershell ionization lines*
  - **SRON/SPEX/TRPB05:** *Differential Emission Measure (DEM) analysis*
  - **SRON/SPEX/TRPB06:** *Active-Region-Loop modelling* (**TBD** by G.H.J. van den Oord)
  - **SRON/SPEX/TRPB07:** *Hot high-gravity LTE atmosphere modelling* (**TBD** by J.Heise)
  - **SRON/SPEX/TRPB08:** *Photo-ionized modelling* (**TBD** by J.S. Kaastra)
- **Instrumental Response and Spectral Simulation:**
  - **SRON/SPEX/TRIS00:** *Overview*
  - **SRON/SPEX/TRIS01:** *EUVE*
  - **SRON/SPEX/TRIS02:** *AXAF*
  - **SRON/SPEX/TRIS03:** *XMM*
  - **SRON/SPEX/TRIS04:** *SAX*
  - **SRON/SPEX/TRIS05:** *ASCA*
- **Cookbook:**
  - **SRON/SPEX/TRCB01:** *Cookbook*

Figure 1.1: Overview of the user level document structure.

Program level

- **SRON/SPEX/TRSW01:** *Introduction to the SPEX software*
- **SRON/SPEX/TRSW02:** *SPEX software description.* Declaration of variables and software level descriptions.
- **SRON/SPEX/TRSW03:** *Installation document.* Test cases, system- and hardware requirements, installation procedure.

Figure 1.2: Overview of the program level document structure.

1.7 Useful addresses

If, after careful examination of the manuals, serious problems remain, or suggestions of improvement arise, please contact one of the persons below:

Rolf Mewe SRON Utrecht, Sorbonnelaan 2 3581 CA Utrecht, The Netherlands	Internet: Fax:	R.Mewe@sron.ruu.nl (+31) (0)30–540860
Jelle Kaastra SRON Utrecht, Sorbonnelaan 2 3581 CA Utrecht, The Netherlands	Internet: Fax:	J.Kaastra@sron.ruu.nl (+31) (0)30–540860

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Chapter 2

Example SPEX session

2.1 Introduction

This chapter presents an example with SPEX. A model will be fitted on a (previously) simulated spectrum of the star II Peg, using the ASCA-SIS instrument. (for more information about the simulation of the spectrum, see document SRON/SPEX/TRCB01). The results of the fit will also be discussed. A schematic overview of the steps to be taken in the SPEX program is presented in Fig. 2.1. Each step will be discussed in a separate section of this chapter.

SPEX can be used in three modes: a *terminal mode*, a *window mode* and a *log file mode*. The example session in this chapter is run in the terminal mode. The same steps may be followed when running SPEX in the window mode. At the end of this chapter, a log file will be presented and discussed. This log file follows the same steps taken in the example, however: automatically. A log file is a series of (previously recorded) SPEX commands that can be executed by SPEX again. To learn more about the log file structure, see chapter 7.

Note: The SPEX menus and program output are displayed here in double lined boxes. The keyboard entries (since this example is run in terminal mode) are denoted with single lined boxes in the texts, commenting the SPEX menus and program output.

2.2 Basic parameters

At the command prompt, type `spex` to start the program.

```
------------------------ SPEX Version  1.00 -------------------------
--------------------------- SPEX main menu ----------------------------
| main | Description                                                   |
-----------------------------------------------------------------------
| QUIT | Exit from SPEX                                                |
| HIDE | Hide (do not hide) menu listings (for experienced user only)|
| LOG  | Log file: save or read log files for commands and output     |
| DIST | Set the source distance                                       |
| GRID | Select default energy grid                                    |
| ELIM | Set energy limits for flux calculations                       |
| VAR  | Define default abundances and line properties etc.            |
| DATA | Read, write, show or modify data (response & obs. spectrum) |
| MOD  | Modify the spectral model                                     |
| PLOT | Plot menu                                                     |
-----------------------------------------------------------------------
Enter your choice [LOG ]:dist
```

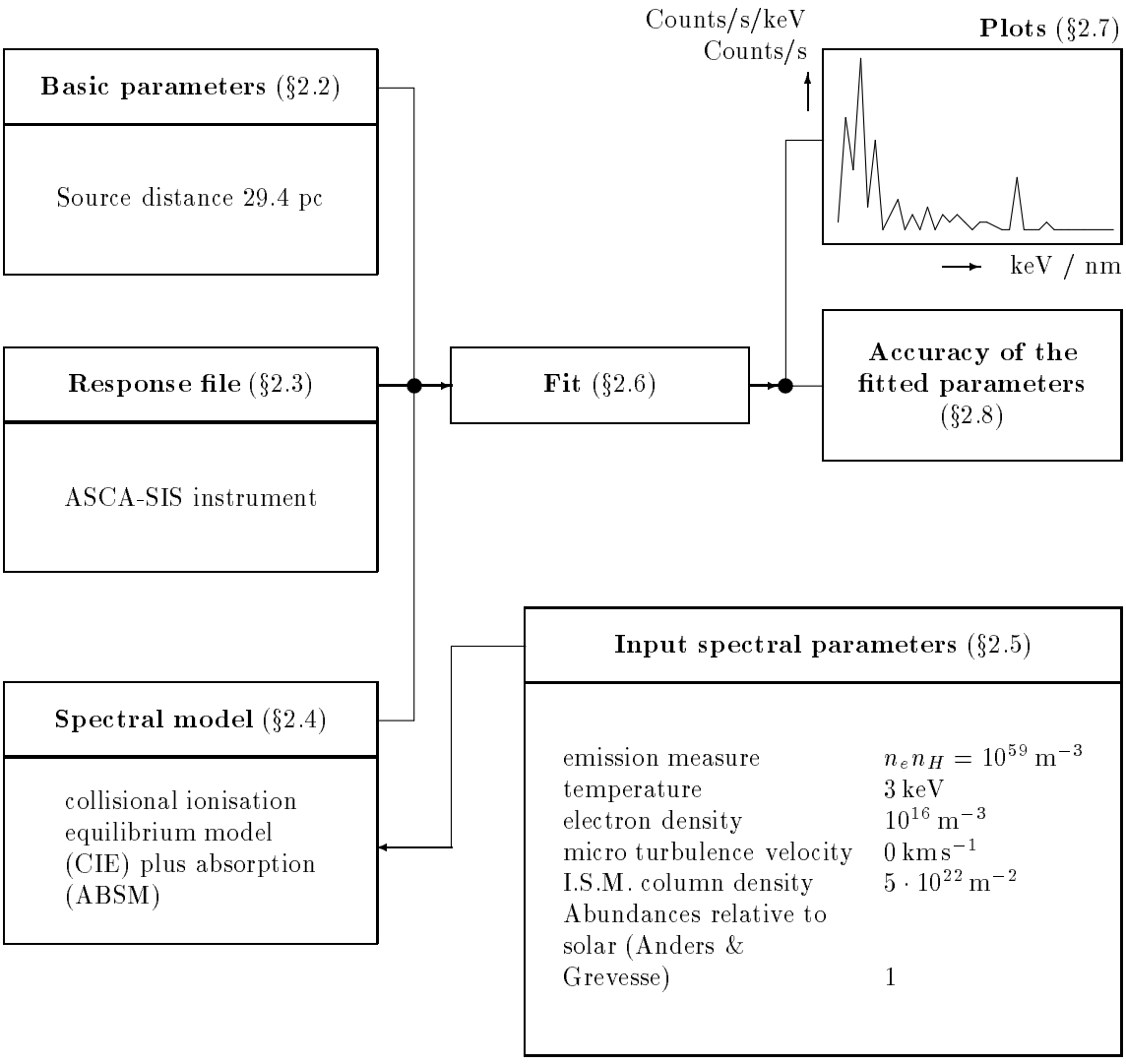

Figure 2.1: Schematic display of example SPEX-session. Each step will be discussed in separate sectiond of this chapter.

Comment: **SPEX** displays a *shortened* version of the main menu. Since there are no data read or models specified, **SPEX** offers only limited possibities. First some basic parameters and units will be set. The distance of the source **must** be specified. This is very important, because SPEX uses luminosities, **not** fluxes, to calculate and fit models, except of course for the observed and simulated spectra. `dist` is entered to set the source distance.

```
------------------------- SPEX Version  1.00 -------------------------
------------------------- SPEX distance menu -------------------------
| dist | Description                                                  |
----------------------------------------------------------------------
| UNIT | Define the unit of your distance scale                       |
| DIST | Enter the value of the distance in your selected units       |
| SHOW | Show the current distance and unit                           |
| MAIN | Back to main menu                                            |
----------------------------------------------------------------------
Enter your choice [UNIT]:
```

Comment: `unit` is entered to define the distance scale.

```
------------------------- SPEX Version  1.00 -------------------------
------------------------- SPEX distance unit menu --------------------
| disu | Description                                                  |
----------------------------------------------------------------------
| SPEX | Distance in 1E22 m                                           |
| AU   | Distance in Astronomical units                               |
| LY   | Distance in light years                                      |
| PC   | Distance in pc                                               |
| KPC  | Distance in kpc                                              |
| MPC  | Distance in Mpc                                              |
| Z    | Cosmological redshift (use H0 = 50, q0=0.5)                  |
| BACK | Back to previous menu                                        |
| MAIN | Back to main menu                                            |
----------------------------------------------------------------------
Enter your choice [SPEX]:pc
```

Comment: The distance scale is taken here in units of parsec (pc), therefore `pc` is entered.

```
------------------------ SPEX Version  1.00 ------------------------
------------------------ SPEX distance menu ------------------------
| dist | Description                                                 |
--------------------------------------------------------------------
| UNIT | Define the unit of your distance scale                      |
| DIST | Enter the value of the distance in your selected units      |
| SHOW | Show the current distance and unit                          |
| MAIN | Back to main menu                                           |
--------------------------------------------------------------------
Enter your choice [DIST]:

Enter the distance in your selected units [324078.]:29.4
```

Comment: `dist` is entered to set the distance of the source in the selected unit. SPEX will ask for a numerical value. In this example `29.4` is entered. The source distance is now 29.4 pc.

```
------------------------ SPEX Version  1.00 ------------------------
------------------------ SPEX distance menu ------------------------
| dist | Description                                                 |
--------------------------------------------------------------------
| UNIT | Define the unit of your distance scale                      |
| DIST | Enter the value of the distance in your selected units      |
| SHOW | Show the current distance and unit                          |
| MAIN | Back to main menu                                           |
--------------------------------------------------------------------
Enter your choice [SHOW]:main
```

Comment: `main` is entered to return to the main menu.

```
------------------------ SPEX Version  1.00 ------------------------
-------------------------- SPEX main menu --------------------------
| main | Description                                                 |
--------------------------------------------------------------------
| QUIT | Exit from SPEX                                              |
| HIDE | Hide (do not hide) menu listings (for experienced user only)|
| LOG  | Log file: save or read log files for commands and output    |
| DIST | Set the source distance                                     |
| GRID | Select default energy grid                                  |
| ELIM | Set energy limits for flux calculations                     |
| VAR  | Define default abundances and line properties etc.          |
| DATA | Read, write, show or modify data (response & obs. spectrum) |
| MOD  | Modify the spectral model                                   |
| PLOT | Plot menu                                                   |
--------------------------------------------------------------------
Enter your choice [GRID]:elim
```

Comment: `elim` is entered to set the energy limits for total flux calculations.

```
------------------------ SPEX Version  1.00 -------------------------
------------ SPEX set energy limits for flux calculation menu -------
| elim | Description                                                  |
---------------------------------------------------------------------
| LOW  | Set lower energy limit (keV)                                 |
| UPP  | Set upper energy limit (keV)                                 |
| MAIN | Back to main menu                                            |
---------------------------------------------------------------------
Enter your choice [LOW ]:

Enter the lower limit in keV [2.]:
```

Comment: The lower value (`low`) is set at `.2` keV.

```
------------------------ SPEX Version  1.00 -------------------------
------------ SPEX set energy limits for flux calculation menu -------
| elim | Description                                                  |
---------------------------------------------------------------------
| LOW  | Set lower energy limit (keV)                                 |
| UPP  | Set upper energy limit (keV)                                 |
| MAIN | Back to main menu                                            |
---------------------------------------------------------------------
Enter your choice [UPP ]:

Enter the upper limit in keV [10.]:12
```

Comment: The upper value (`upp`) is set at `12` keV.

```
------------------------ SPEX Version  1.00 -------------------------
------------ SPEX set energy limits for flux calculation menu -------
| elim | Description                                                  |
---------------------------------------------------------------------
| LOW  | Set lower energy limit (keV)                                 |
| UPP  | Set upper energy limit (keV)                                 |
| MAIN | Back to main menu                                            |
---------------------------------------------------------------------
Enter your choice [MAIN]:
```

Comment: `main` is entered to return to the main menu.

2.3 Response file

```
------------------------ SPEX Version  1.00 -------------------------
-------------------------- SPEX main menu ---------------------------
| main | Description                                                  |
---------------------------------------------------------------------
| QUIT | Exit from SPEX                                               |
| HIDE | Hide (do not hide) menu listings (for experienced user only) |
| LOG  | Log file: save or read log files for commands and output     |
| DIST | Set the source distance                                      |
| GRID | Select default energy grid                                   |
| ELIM | Set energy limits for flux calculations                      |
| VAR  | Define default abundances and line properties etc.           |
| DATA | Read, write, show or modify data (response & obs. spectrum)  |
| MOD  | Modify the spectral model                                    |
| PLOT | Plot menu                                                    |
---------------------------------------------------------------------
Enter your choice [VAR ]:grid
```

Comment: `grid` is entered to define the energy grid on which the calculation will be done.

```
------------------------ SPEX Version  1.00 -------------------------
----------------- SPEX model energy grid selection menu --------------
| grid | Description                                                  |
---------------------------------------------------------------------
| LIN  | Linear energy grid                                           |
| LOG  | Logarithmic energy grid                                      |
| FILE | Input your own grid from a file                              |
| DATA | Input the grid of a response matrix                          |
| SAVE | Save the current energy grid to a file                       |
| MAIN | Back to main menu                                            |
---------------------------------------------------------------------
Enter your choice [LOG ]:data
```

Comment: This example uses a simulation of the *ASCA-SIS* data, therefore a compatible energy grid must be used. A response matrix of the *ASCA-SIS* instrument is available (see document SRON/-SPEX/TRIS05) and `data` is entered to read it.

```
------------------------ SPEX Version  1.00 -------------------------
-------------- SPEX model energy grid from response matrix menu ------
| gdat | Description                                                   |
-----------------------------------------------------------------------
| NAME | Set file name of response matrix with energy grid             |
| READ | Read the file with the energy grid                            |
| BACK | Back to previous menu                                         |
| MAIN | Back to main menu                                             |
-----------------------------------------------------------------------
Enter your choice [NAME]:

Enter response matrix (without .res extension) [spex]:iipeg3a
```

Comment: `name` is entered to define the name of the file containing the response matrix. SPEX asks for a name and `iipeg3a` is entered.

```
------------------------ SPEX Version  1.00 -------------------------
-------------- SPEX model energy grid from response matrix menu ------
| gdat | Description                                                   |
-----------------------------------------------------------------------
| NAME | Set file name of response matrix with energy grid             |
| READ | Read the file with the energy grid                            |
| BACK | Back to previous menu                                         |
| MAIN | Back to main menu                                             |
-----------------------------------------------------------------------
Enter your choice [READ]:

Your energy grid contains  989 bins.
Start energy:    0.19886     keV
End   energy:     11.993     keV
```

Comment: `read` is entered to read the response matrix. After the file is read and processed, SPEX displays the start and end energies of the energy grid and returns to the main menu.

```
------------------------- SPEX Version  1.00 -------------------------
--------------------------- SPEX main menu ---------------------------
| main | Description                                                  |
-----------------------------------------------------------------------
| QUIT | Exit from SPEX                                               |
| HIDE | Hide (do not hide) menu listings (for experienced user only) |
| LOG  | Log file: save or read log files for commands and output     |
| DIST | Set the source distance                                      |
| GRID | Select default energy grid                                   |
| ELIM | Set energy limits for flux calculations                      |
| VAR  | Define default abundances and line properties etc.           |
| DATA | Read, write, show or modify data (response & obs. spectrum)  |
| MOD  | Modify the spectral model                                    |
| PLOT | Plot menu                                                    |
-----------------------------------------------------------------------
Enter your choice [ELIM]:data
```

Comment: Back in the main menu, `data` is selected to read the observed spectrum and the response file.

```
------------------------- SPEX Version  1.00 -------------------------
--------------------------- SPEX data menu ---------------------------
| dat  | Description                                                  |
-----------------------------------------------------------------------
| FORM | Set the format of the data files (binary or ascii)           |
| TYPE | Type of data to be read or written (res, spo or res & spo)   |
| COMB | How are the new data to be combined with the old data        |
| READ | Read new data set (be sure FORM, TYPE and COMB are correct)  |
| WRIT | Save the current data set (be sure FORM & TYPE are correct)  |
| DMOD | Modify, rebin or optimise the current data set               |
| SHOW | Show the current data set                                    |
| MAIN | Back to main menu                                            |
-----------------------------------------------------------------------
Enter your choice [SHOW]:read
```

Comment: `read` is entered to read a new data set.

```
------------------------ SPEX Version  1.00 ------------------------
------------------------- SPEX data read menu ----------------------
| read | Description                                                 |
-----------------------------------------------------------------------
| RNAM | Change file name containing the response matrix             |
| SNAM | Change file name containing the spectrum                    |
| READ | Read the data set from named file                           |
| BACK | Back to previous menu                                       |
| MAIN | Back to main menu                                           |
-----------------------------------------------------------------------
Enter your choice [RNAM]:

Give file name (without .res or .ras extension) [iipeg3a]:
```

Comment: The name of the file containing the response matrix is set by entering `rnam` and `iipeg3a`.

```
------------------------ SPEX Version  1.00 ------------------------
------------------------- SPEX data read menu ----------------------
| read | Description                                                 |
-----------------------------------------------------------------------
| RNAM | Change file name containing the response matrix             |
| SNAM | Change file name containing the spectrum                    |
| READ | Read the data set from named file                           |
| BACK | Back to previous menu                                       |
| MAIN | Back to main menu                                           |
-----------------------------------------------------------------------
Enter your choice [SNAM]:

Give file name (without .spo or .spa extension) [spex]:iipeg3a
```

Comment: The name of the file containing the spectrum is set by entering `snam` and `iipeg3a`.

```
------------------------ SPEX Version  1.00 ------------------------
------------------------- SPEX data read menu ----------------------
| read | Description                                                 |
-----------------------------------------------------------------------
| RNAM | Change file name containing the response matrix             |
| SNAM | Change file name containing the spectrum                    |
| READ | Read the data set from named file                           |
| BACK | Back to previous menu                                       |
| MAIN | Back to main menu                                           |
-----------------------------------------------------------------------
Enter your choice [READ]:
```

Comment: `read` is entered to read the complete data set.

```
------------------------ SPEX Version  1.00 -------------------------
--------------------------- SPEX data menu ----------------------------
| dat  | Description                                                    |
-----------------------------------------------------------------------
| FORM | Set the format of the data files (binary or ascii)             |
| TYPE | Type of data to be read or written (res, spo or res & spo)     |
| COMB | How are the new data to be combined with the old data          |
| READ | Read new data set (be sure FORM, TYPE and COMB are correct)    |
| WRIT | Save the current data set (be sure FORM & TYPE are correct)    |
| DMOD | Modify, rebin or optimise the current data set                 |
| SHOW | Show the current data set                                      |
| MAIN | Back to main menu                                              |
-----------------------------------------------------------------------
Enter your choice [SHOW]:show
```

Comment: `show` is entered to show the characteristics of the data that were just read.

```
Your energy grid contains  989 bins.
 Start energy:    0.19886     keV
 End   energy:     11.993     keV
 Latest spectral data file            : iipeg3a
 Latest spectral response file        : iipeg3a
 Number of photon model energy bins   :      989
 Number of data channels              :      230
 Number of response groups            :      989
 Number of non-zero response elements :     8487
 Photon model energy range (keV)      :    0.19886        11.993
 Data energy range (keV)              :    0.25523        12.047
 Net source count rate (counts/s)     :    0.62613     +/-    3.97201E-03
 Net source counts                    :    25045 +/-      159
 Background count rate subtracted(c/s):    4.40611E-03
 Background counts subtracted         :      176
 Average integration time per channel :     40000.     s
 Minimum integration time per channel :     40000.     s
 Maximum integration time per channel :     40000.     s
 Aver. exposure rat. source/background:    0.10000     s
 Min. exposure ratio source/background:    0.10000     s
 Max. exposure ratio source/background:    0.10000     s
```

Comment: The menu returns after the data have been displayed.

```
------------------------ SPEX Version  1.00 ------------------------
-------------------------- SPEX data menu --------------------------
| dat  | Description                                                 |
-----------------------------------------------------------------------
| FORM | Set the format of the data files (binary or ascii)          |
| TYPE | Type of data to be read or written (res, spo or res & spo)  |
| COMB | How are the new data to be combined with the old data       |
| READ | Read new data set (be sure FORM, TYPE and COMB are correct) |
| WRIT | Save the current data set (be sure FORM & TYPE are correct) |
| DMOD | Modify, rebin or optimise the current data set              |
| SHOW | Show the current data set                                   |
| MAIN | Back to main menu                                           |
-----------------------------------------------------------------------
Enter your choice [SHOW]:main
```

Comment: `main` is entered to return to the main menu.

2.4 Spectral model

```
------------------------ SPEX Version  1.00 ------------------------
-------------------------- SPEX main menu --------------------------
| main | Description                                                 |
-----------------------------------------------------------------------
| QUIT | Exit from SPEX                                              |
| HIDE | Hide (do not hide) menu listings (for experienced user only)|
| LOG  | Log file: save or read log files for commands and output     |
| DIST | Set the source distance                                     |
| GRID | Select default energy grid                                  |
| ELIM | Set energy limits for flux calculations                     |
| VAR  | Define default abundances and line properties etc.          |
| DATA | Read, write, show or modify data (response & obs. spectrum) |
| MOD  | Modify the spectral model                                   |
| PLOT | Plot menu                                                   |
-----------------------------------------------------------------------
Enter your choice [MOD ]:
```

Comment: `mod` is entered to specify the spectral model.

```
------------------------- SPEX Version  1.00 -------------------------
--------------------------- SPEX model menu ---------------------------
| mod   | Description                                                  |
-----------------------------------------------------------------------
| ADD   | Define an additive component                                 |
| SHOW  | Show the current model                                       |
| BACK  | Back to main menu                                            |
-----------------------------------------------------------------------
Enter your choice [ADD ]:
```

Comment: First, `add` is entered to define an additive component

```
------------------------- SPEX Version  1.00 -------------------------
-------------------- Define an additive component --------------------
| moda  | Description                                                  |
-----------------------------------------------------------------------
| POW   | Simple power law                                             |
| DELT  | Delta line                                                   |
| CIE   | Collisional ionisation equilibrium model                     |
| NEIJ  | NEI model: discontinuous temperature jump                    |
| SED   | SNR model: Sedov (adiabatic)                                 |
| CHEV  | SNR model: Chevalier (adiabatic, reverse shock)              |
| HAM   | SNR model: Hamilton (adiabatic, reverse shock, clumps)       |
| SOLI  | SNR model: Solinger et al. (isothermal)                      |
| BAND  | SNR model: Band (isothermal or isentropic, reverse shock)    |
| DEM   | DEM model: differential emission measure analysis            |
| MBB   | Modified black body spectrum (MBB)                           |
| GAUS  | Gaussian line                                                |
| BB    | Black body spectrum                                          |
| BACK  | BACK to previous menu                                        |
-----------------------------------------------------------------------
Enter your choice [POW ]:cie

You have defined  1 additive components.
```

Comment: SPEX shows the list of available additive model components. See chapter 4 of this manual and SRON/SPEX/TRCB01 for more information about the spectral model components. This example will use the *collisional ionization equilibrium model*, therefore `cie` is entered. SPEX shows the number of additive components that are currently defined.

```
------------------------- SPEX Version  1.00 -------------------------
--------------------- Define an additive component ---------------------
| moda | Description                                                    |
----------------------------------------------------------------------
| POW  | Simple power law                                               |
| DELT | Delta line                                                     |
| CIE  | Collisional ionisation equilibrium model                       |
| NEIJ | NEI model: discontinuous temperature jump                      |
| SED  | SNR model: Sedov (adiabatic)                                   |
| CHEV | SNR model: Chevalier (adiabatic, reverse shock)                |
| HAM  | SNR model: Hamilton (adiabatic, reverse shock, clumps)         |
| SOLI | SNR model: Solinger et al. (isothermal)                        |
| BAND | SNR model: Band (isothermal or isentropic, reverse shock)      |
| DEM  | DEM model: differential emission measure analysis              |
| MBB  | Modified black body spectrum (MBB)                             |
| GAUS | Gaussian line                                                  |
| BB   | Black body spectrum                                            |
| BACK | BACK to previous menu                                          |
----------------------------------------------------------------------
Enter your choice [BACK]:
```

Comment: `back` is enterted to return to the model menu.

```
------------------------- SPEX Version  1.00 -------------------------
-------------------------- SPEX model menu ---------------------------
| mod  | Description                                                   |
----------------------------------------------------------------------
| ADD  | Define an additive component                                  |
| MUL  | Define a multiplicative or redshift component                 |
| DADD | Delete an additive component                                  |
| SHOW | Show the current model                                        |
| BACK | Back to main menu                                             |
----------------------------------------------------------------------
Enter your choice [MUL ]:
```

Comment: `mul` is entered to define a multiplicative component.

```
------------------------ SPEX Version  1.00 -------------------------
-------------- Define a multiplicative or redshift component ---------
| modb | Description                                                   |
---------------------------------------------------------------------
| REDS | Redshift component                                            |
| ABSM | Absorption component (Morrison & McCammon)                    |
| EUVE | Absorption component (EUVE)                                   |
| HOT  | Absorption component (hot CIE medium)                         |
| BACK | Back to previous menu                                         |
---------------------------------------------------------------------
Enter your choice [REDS]:absm

You have defined  1 multiplicative components.
```

Comment: SPEX shows the list of available multiplicative components. See chapter 4 of this manual and SRON/SPEX/TRCB01 for more information on the spectral model components. This example uses the absorption cross sections of *Morrison & McCammon* (1983), therefore `absm` is entered. SPEX shows the number of multiplicative components that are currently defined.

```
------------------------ SPEX Version  1.00 -------------------------
-------------- Define a multiplicative or redshift component ---------
| modb | Description                                                   |
---------------------------------------------------------------------
| REDS | Redshift component                                            |
| ABSM | Absorption component (Morrison & McCammon)                    |
| EUVE | Absorption component (EUVE)                                   |
| HOT  | Absorption component (hot CIE medium)                         |
| BACK | Back to previous menu                                         |
---------------------------------------------------------------------
Enter your choice [BACK]:
```

Comment: `back` is entered to return to the model menu.

```
------------------------ SPEX Version  1.00 -------------------------
--------------------------- SPEX model menu --------------------------
| mod  | Description                                                  |
---------------------------------------------------------------------
| ADD  | Define an additive component                                 |
| MUL  | Define a multiplicative or redshift component                |
| DADD | Delete an additive component                                 |
| DMUL | Delete a multiplicative or redshift component                |
| REL  | Set relation additive & multiplicative components            |
| SHOW | Show the current model                                       |
| BACK | Back to main menu                                            |
---------------------------------------------------------------------
Enter your choice [REL ]:
```

Comment: The spectral model is now defined. `rel` is entered to set the relations between the additive and multiplicative components.

```
------------------------ SPEX Version  1.00 -------------------------
--------- Define relations additive and multiplicative components ----
| mode | Description                                                  |
-------------------------------------------------------------------------
| A01  | Define relations for additive component  1                   |
| SAME | Define the same dependence for all additive components       |
| BACK | Back to previous menu                                        |
-------------------------------------------------------------------------
Enter your choice [SAME]:

Enter the dependency [ 0, 0, 0, 0, 0, 0, 0, 0]:1
```

Comment: SPEX shows the relations between the current spectral model components. In this example, all components need to have the same dependency. thus `same` is entered. Spex asks for a numerical input value and `1` is entered. This indicates that the `cie` component will be multiplied with the multiplicative component (the `absm` component). If more multiplicative components had been defined, their dependencies are specified as well, e.g. 3,1,2 in the case of 3 multiplicative components. This would mean that first the third, then the first and finally the the second multiplicative component would be applied to the selected additive component.

```
------------------------ SPEX Version  1.00 -------------------------
--------------------------- SPEX model menu ---------------------------
| mod  | Description                                                  |
-------------------------------------------------------------------------
| ADD  | Define an additive component                                 |
| MUL  | Define a multiplicative or redshift component                |
| DADD | Delete an additive component                                 |
| DMUL | Delete a multiplicative or redshift component                |
| REL  | Set relation additive & multiplicative components            |
| SHOW | Show the current model                                       |
| BACK | Back to main menu                                            |
-------------------------------------------------------------------------
Enter your choice [SHOW]:
```

Comment: `show` is entered to get an overview of the spectral model.

```
-------------------------------------------------------------------------
 Number of multiplicative components:   1
    Nr.   1: absm
 Number of additive components      :   1
    Nr.   1: cie [ 1, 0, 0, 0, 0, 0, 0, 0]
```

Comment: SPEX shows the components and their relations.

```
------------------------- SPEX Version  1.00 -------------------------
--------------------------- SPEX model menu ---------------------------
| mod  | Description                                                   |
---------------------------------------------------------------------
| ADD  | Define an additive component                                  |
| MUL  | Define a multiplicative or redshift component                 |
| DADD | Delete an additive component                                  |
| DMUL | Delete a multiplicative or redshift component                 |
| REL  | Set relation additive & multiplicative components             |
| SHOW | Show the current model                                        |
| BACK | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [SHOW]:back
```

Comment: back is entered to return to the main menu.

2.5 Input spectral parameters

```
------------------------- SPEX Version  1.00 -------------------------
--------------------------- SPEX main menu ----------------------------
| main | Description                                                   |
---------------------------------------------------------------------
| QUIT | Exit from SPEX                                                |
| HIDE | Hide (do not hide) menu listings (for experienced user only)  |
| LOG  | Log file: save or read log files for commands and output      |
| DIST | Set the source distance                                       |
| GRID | Select default energy grid                                    |
| ELIM | Set energy limits for flux calculations                       |
| VAR  | Define default abundances and line properties etc.            |
| DATA | Read, write, show or modify data (response & obs. spectrum)   |
| MOD  | Modify the spectral model                                     |
| PAR  | Modify the current model parameters                           |
| CALC | Evaluate the current spectral model                           |
| SIM  | Simulate a spectrum using current model & detector            |
| FIT  | Spectral fitting, error search etc.                           |
| ASC  | Output of SPEX model properties to ascii file or screen       |
| PLOT | Plot menu                                                     |
---------------------------------------------------------------------
Enter your choice [PAR ]:
```

Comment: All spectral model components are defined with default values at program startup. par is entered to modify some spectral model parameters of the current spectral model.

```
------------------------ SPEX Version  1.00 -------------------------
------------------ Define or modify spectral parameters --------------
| par  | Description                                                   |
---------------------------------------------------------------------
| COMP | Select the spectral component                                 |
| PARA | Select the parameter for the current component                |
| VAL  | Set new value of the parameter                                |
| STAT | Set new status of the parameter                               |
| STEP | Set new step for the parameter                                |
| LOW  | Set new minimum for the parameter                             |
| UPP  | Set new maximum for the parameter                             |
| SHOW | Show the current parameters                                   |
| RCOR | Show the correlations between the fitted parameters           |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [COMP]:
```

Comment: First a spectral component needs to be selected, therefore `comp` is selected.

```
------------------------ SPEX Version  1.00 -------------------------
---------------------- Select a spectral component ------------------
| comp | Description                                                   |
---------------------------------------------------------------------
| A01  | Additive component  1                                         |
| M01  | Multiplicative component  1                                   |
---------------------------------------------------------------------
Enter your choice [A01 ]:
```

Comment: The spectral parameters of the additive component will be modified first. `a01` is entered to select the additive component #1 (i.e. CIE).

```
------------------------ SPEX Version  1.00 -------------------------
------------------ Define or modify spectral parameters --------------
| par  | Description                                                   |
---------------------------------------------------------------------
| COMP | Select the spectral component                                 |
| PARA | Select the parameter for the current component                |
| VAL  | Set new value of the parameter                                |
| STAT | Set new status of the parameter                               |
| STEP | Set new step for the parameter                                |
| LOW  | Set new minimum for the parameter                             |
| UPP  | Set new maximum for the parameter                             |
| SHOW | Show the current parameters                                   |
| RCOR | Show the correlations between the fitted parameters           |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [PARA]:
```

Comment: `para` is entered to select a parameter from the current component (CIE).

```
------------------------ SPEX Version  1.00 -------------------------
------------------- Select a spectral parameter (CIE model) ----------
| scie | Description                                                   |
---------------------------------------------------------------------
| NORM | Normalisation = ne nH V (1E64/m**3)                           |
| T    | Electron temperature (keV)                                    |
| ED   | Electron density (1E20 /m**3)                                 |
| IT   | Ion temperature (keV)                                         |
| VMIC | Micro turbulence velocity (km/s)                              |
| 02   | Abundance He (Z=2)                                            |
| ..   |    ...   (shortened)                                          |
| 30   | Abundance Zn (Z=30)                                           |
---------------------------------------------------------------------
Enter your choice [NORM]:
```

Comment: `norm` is entered to select the normalization parameter

```
------------------------ SPEX Version  1.00 -------------------------
------------------ Define or modify spectral parameters --------------
| par  | Description                                                   |
---------------------------------------------------------------------
| COMP | Select the spectral component                                 |
| PARA | Select the parameter for the current component                |
| VAL  | Set new value of the parameter                                |
| STAT | Set new status of the parameter                               |
| STEP | Set new step for the parameter                                |
| LOW  | Set new minimum for the parameter                             |
| UPP  | Set new maximum for the parameter                             |
| SHOW | Show the current parameters                                   |
| RCOR | Show the correlations between the fitted parameters           |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [VAL ]:

add. comp.  1 (cie ): ne nH V (1E64/m**3)  (type = 0) [1.]:1e-5
```

Comment: In this example only the value of the selected parameter needs to be nodified, thus `val` is selected and the new value is entered: `1e-5` (i.e. 10^{59} m^{-3}).

```
------------------------- SPEX Version  1.00 -------------------------
------------------ Define or modify spectral parameters --------------
| par  | Description                                                   |
---------------------------------------------------------------------
| COMP | Select the spectral component                                 |
| PARA | Select the parameter for the current component                |
| VAL  | Set new value of the parameter                                |
| STAT | Set new status of the parameter                               |
| STEP | Set new step for the parameter                                |
| LOW  | Set new minimum for the parameter                             |
| UPP  | Set new maximum for the parameter                             |
| SHOW | Show the current parameters                                   |
| RCOR | Show the correlations between the fitted parameters           |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [VAL ]:para
```

Comment: `para` is entered to select another parameter from the current spectral component (CIE).

```
------------------------- SPEX Version  1.00 -------------------------
------------------- Select a spectral parameter (CIE model) ----------
| scie | Description                                                  |
---------------------------------------------------------------------
| NORM | Normalisation = ne nH V (1E64/m**3)                          |
| T    | Electron temperature (keV)                                   |
| ED   | Electron density (1E20 /m**3)                                |
| IT   | Ion temperature (keV)                                        |
| VMIC | Micro turbulence velocity (km/s)                             |
| 02   | Abundance He (Z=2)                                           |
| ..   |    ...  (shortened)                                          |
| 30   | Abundance Zn (Z=30)                                          |
---------------------------------------------------------------------
Enter your choice [NORM]:t
```

Comment: The electron temperature is selected by entering `t` .

```
------------------------- SPEX Version  1.00 -------------------------
------------------ Define or modify spectral parameters --------------
 | par  | Description                                                  |
 ---------------------------------------------------------------------
 | COMP | Select the spectral component                                |
 | PARA | Select the parameter for the current component               |
 | VAL  | Set new value of the parameter                               |
 | STAT | Set new status of the parameter                              |
 | STEP | Set new step for the parameter                               |
 | LOW  | Set new minimum for the parameter                            |
 | UPP  | Set new maximum for the parameter                            |
 | SHOW | Show the current parameters                                  |
 | RCOR | Show the correlations between the fitted parameters          |
 | MAIN | Back to main menu                                            |
 ---------------------------------------------------------------------
 Enter your choice [VAL ]:

add. comp.  1 (cie ): Temperature (keV)    (type = 2) [1.]:5
```

Comment: The value is modified by entering `val` and the new value: `5` (i.e. 5 keV).

```
- ------------------ Define or modify spectral parameters --------------
 | par  | Description                                                  |
 ---------------------------------------------------------------------
 | COMP | Select the spectral component                                |
 | PARA | Select the parameter for the current component               |
 | VAL  | Set new value of the parameter                               |
 | STAT | Set new status of the parameter                              |
 | STEP | Set new step for the parameter                               |
 | LOW  | Set new minimum for the parameter                            |
 | UPP  | Set new maximum for the parameter                            |
 | SHOW | Show the current parameters                                  |
 | RCOR | Show the correlations between the fitted parameters          |
 | MAIN | Back to main menu                                            |
 ---------------------------------------------------------------------
 Enter your choice [VAL ]:para
```

Comment: The same steps are followed to set the values of ion temperature and electron density at 1 keV (`1`) and 10^{16} m^{-3} (`1e-4`) respectively.

```
------------------------ SPEX Version  1.00 -------------------------
------------------- Select a spectral parameter (CIE model) ----------
| scie | Description                                                   |
---------------------------------------------------------------------
| NORM | Normalisation = ne nH V (1E64/m**3)                           |
| T    | Electron temperature (keV)                                    |
| ED   | Electron density (1E20 /m**3)                                 |
| IT   | Ion temperature (keV)                                         |
| VMIC | Micro turbulence velocity (km/s)                              |
| 02   | Abundance He (Z=2)                                            |
| ..   |    ...  (shortened)                                           |
| 30   | Abundance Zn (Z=30)                                           |
---------------------------------------------------------------------
Enter your choice [NORM]:it
```

Comment: The ion temperature is selected by entering `it` .

```
------------------------ SPEX Version  1.00 -------------------------
------------------ Define or modify spectral parameters --------------
| par  | Description                                                   |
---------------------------------------------------------------------
| COMP | Select the spectral component                                 |
| PARA | Select the parameter for the current component                |
| VAL  | Set new value of the parameter                                |
| STAT | Set new status of the parameter                               |
| STEP | Set new step for the parameter                                |
| LOW  | Set new minimum for the parameter                             |
| UPP  | Set new maximum for the parameter                             |
| SHOW | Show the current parameters                                   |
| RCOR | Show the correlations between the fitted parameters           |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [VAL ]:

add. comp.  1 (cie ): Ion temp. (keV)      (type = 3) [1.]:
```

Comment: The value is modified by entering `val` and the value `1` (i.e. 1 keV).

```
------------------------- SPEX Version  1.00 -------------------------
------------------ Define or modify spectral parameters --------------
| par  | Description                                                   |
---------------------------------------------------------------------
| COMP | Select the spectral component                                 |
| PARA | Select the parameter for the current component                |
| VAL  | Set new value of the parameter                                |
| STAT | Set new status of the parameter                               |
| STEP | Set new step for the parameter                                |
| LOW  | Set new minimum for the parameter                             |
| UPP  | Set new maximum for the parameter                             |
| SHOW | Show the current parameters                                   |
| RCOR | Show the correlations between the fitted parameters           |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [VAL ]:para
```

Comment: This multiplicative component only has one parameter: the column density.

```
------------------------- SPEX Version  1.00 -------------------------
------------------- Select a spectral parameter (CIE model) ----------
| scie | Description                                                  |
---------------------------------------------------------------------
| NORM | Normalisation = ne nH V (1E64/m**3)                          |
| T    | Electron temperature (keV)                                   |
| ED   | Electron density (1E20 /m**3)                                |
| IT   | Ion temperature (keV)                                        |
| VMIC | Micro turbulence velocity (km/s)                             |
| 02   | Abundance He (Z=2)                                           |
| ..   |          (shortened)
| 30   | Abundance Zn (Z=30)                                          |
---------------------------------------------------------------------
Enter your choice [NORM]:ed
```

Comment: The electron density is selected by entering ed .

```
------------------------- SPEX Version  1.00 -------------------------
------------------ Define or modify spectral parameters --------------
| par  | Description                                                   |
---------------------------------------------------------------------
| COMP | Select the spectral component                                 |
| PARA | Select the parameter for the current component                |
| VAL  | Set new value of the parameter                                |
| STAT | Set new status of the parameter                               |
| STEP | Set new step for the parameter                                |
| LOW  | Set new minimum for the parameter                             |
| UPP  | Set new maximum for the parameter                             |
| SHOW | Show the current parameters                                   |
| RCOR | Show the correlations between the fitted parameters           |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [VAL ]:

add. comp.  1 (cie ): El. dens (1E20/m**3) (type = 2) [1.E-14]:1e-4
```

Comment: The value is modified by entering `val` and the value: `1e-4` (i.e. 10^{16} m^{-3}).

```
------------------------- SPEX Version  1.00 -------------------------
------------------ Define or modify spectral parameters --------------
| par  | Description                                                   |
---------------------------------------------------------------------
| COMP | Select the spectral component                                 |
| PARA | Select the parameter for the current component                |
| VAL  | Set new value of the parameter                                |
| STAT | Set new status of the parameter                               |
| STEP | Set new step for the parameter                                |
| LOW  | Set new minimum for the parameter                             |
| UPP  | Set new maximum for the parameter                             |
| SHOW | Show the current parameters                                   |
| RCOR | Show the correlations between the fitted parameters           |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [VAL ]:comp
```

Comment: Now the parameters of the multiplicative component will be modified. `comp` is entered to select a new spectral component.

```
------------------------- SPEX Version  1.00 -------------------------
----------------------- Select a spectral component ------------------
| comp | Description                                                   |
-----------------------------------------------------------------------
| A01  | Additive component  1                                         |
| M01  | Multiplicative component  1                                   |
-----------------------------------------------------------------------
Enter your choice [A01 ]:m01
```

Comment: m01 is entered to select the multiplicative component #1 (i.e. ABSM).

```
------------------------- SPEX Version  1.00 -------------------------
----------------- Define or modify spectral parameters --------------
| par  | Description                                                   |
-----------------------------------------------------------------------
| COMP | Select the spectral component                                 |
| PARA | Select the parameter for the current component                |
| VAL  | Set new value of the parameter                                |
| STAT | Set new status of the parameter                               |
| STEP | Set new step for the parameter                                |
| LOW  | Set new minimum for the parameter                             |
| UPP  | Set new maximum for the parameter                             |
| SHOW | Show the current parameters                                   |
| RCOR | Show the correlations between the fitted parameters           |
| MAIN | Back to main menu                                             |
-----------------------------------------------------------------------
Enter your choice [PARA]:
```

Comment: This multiplicative component only has one parameter: the column density.

```
------------------------- SPEX Version  1.00 -------------------------
---------------- Select a spectral parameter (absorption M&M) --------
| sabs | Description                                                   |
-----------------------------------------------------------------------
| NH   | Hydrogen column density (1E28 /m**2 = 1E24 /cm**2)            |
-----------------------------------------------------------------------
Enter your choice [NH  ]:
```

Comment: NH is entered to select the hydrogen column density.

```
------------------------- SPEX Version  1.00 -------------------------
------------------ Define or modify spectral parameters --------------
| par  | Description                                                   |
---------------------------------------------------------------------
| COMP | Select the spectral component                                 |
| PARA | Select the parameter for the current component                |
| VAL  | Set new value of the parameter                                |
| STAT | Set new status of the parameter                               |
| STEP | Set new step for the parameter                                |
| LOW  | Set new minimum for the parameter                             |
| UPP  | Set new maximum for the parameter                             |
| SHOW | Show the current parameters                                   |
| RCOR | Show the correlations between the fitted parameters           |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [VAL ]:

mul. comp.  1 (absm): Column (1E28/m**2)   (type = 2) [1.E-04]:5e-6
```

Comment: This multiplicative component only has one parameter: the column density. Therefore `val` can be selected without selecting the parameter first. The new value is set at $5\ .\ 10^{22}\ \mathrm{m}^{-2}$ by entering `5e-6` .

```
------------------------- SPEX Version  1.00 -------------------------
------------------ Define or modify spectral parameters --------------
| par  | Description                                                   |
---------------------------------------------------------------------
| COMP | Select the spectral component                                 |
| PARA | Select the parameter for the current component                |
| VAL  | Set new value of the parameter                                |
| STAT | Set new status of the parameter                               |
| STEP | Set new step for the parameter                                |
| LOW  | Set new minimum for the parameter                             |
| UPP  | Set new maximum for the parameter                             |
| SHOW | Show the current parameters                                   |
| RCOR | Show the correlations between the fitted parameters           |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [VAL ]:main
```

Comment: `main` is selected to return to the main menu.

2.6 Fit of the parameters

```
------------------------- SPEX Version  1.00 -------------------------
---------------------------- SPEX main menu ----------------------------
| main | Description                                                    |
----------------------------------------------------------------------
| QUIT | Exit from SPEX                                                 |
| HIDE | Hide (do not hide) menu listings (for experienced user only)|
| LOG  | Log file: save or read log files for commands and output       |
| DIST | Set the source distance                                        |
| GRID | Select default energy grid                                     |
| ELIM | Set energy limits for flux calculations                        |
| VAR  | Define default abundances and line properties etc.             |
| DATA | Read, write, show or modify data (response & obs. spectrum)    |
| MOD  | Modify the spectral model                                      |
| PAR  | Modify the current model parameters                            |
| CALC | Evaluate the current spectral model                            |
| SIM  | Simulate a spectrum using current model & detector             |
| FIT  | Spectral fitting, error search etc.                            |
| ASC  | Output of SPEX model properties to ascii file or screen        |
| PLOT | Plot menu                                                      |
----------------------------------------------------------------------
Enter your choice [CALC]:fit
```

Comment: `fit` is entered to fit the currently defined spectral model to the spectral data.

```
------------------------- SPEX Version  1.00 -------------------------
---------------------------- SPEX fit menu -----------------------------
| fit  | Description                                                    |
----------------------------------------------------------------------
| METH | change the spectral fitting method                             |
| RUN  | fit the parameters using current data & model                  |
| ERR  | determine error bounds on parameters                           |
| STEP | do a grid search                                               |
| MAIN | Back to main menu                                              |
----------------------------------------------------------------------
Enter your choice [RUN ]:
----------------------------------------------------------------------
```

Comment: The parameters will be fitted with the default method at program startup (Levenberg-Marquardt & linear scalings). Therefore `run` may be entered without setting the fitting method first.

```
------------------------------------------------------------------------
iter lamda    chisq    param  2   param 35
  0 1.E-02   2539.4395   5.00      5.000E-06
  0 1.E-03   2386.5146   1.96      4.572E-05
  0 1.E-04    350.2993   2.63      3.936E-05
  0 1.E-05    222.2223   2.89      1.514E-05
  0 1.E-06    221.7196   2.91      1.228E-05
  1 1.E-05    221.7196   2.91      1.228E-05
  2 1.E-04    221.7196   2.91      1.228E-05
  3 1.E-03    221.7196   2.91      1.228E-05
  4 0.E+00    221.7196   2.91      1.228E-05
------------------------------------------------------------------------
```

Comment: SPEX fits the spectral model with the spectral data iteratively. The number of successive trials to improve the fit is shown as "iter". Convergence is assumed to occur at iter=4. After each iteration, SPEX shows the fit parameter λ (described in Press et al. 1992), the χ^2 value and the value of the free parameters of the current spectral model. In this example `param 2` is the temperature (keV) and `param 35` the column density. The numbers denote the number with respect to the total number of spectral model parameters in the current spectral model. Note that normalization parameters are not shown. If there would have been more than 5 free parameters in the current spectral model, only the first five of these would be shown during the fitting procedure.

NOTE: Due to improvements in the atomic physics used in SPEX, minor differences may occur between the fits as presented in this manual and the fits that are made with your current implementation of SPEX. Always check the version number that is used.

```
------------------------------------------------------------------------------
 mod  nr t parameter with unit     value     st      step   minimum   maximum

 cie   1 0 ne nH V (1E64/m**3)   9.81741E-06  1  1.00E-03 -1.00E+20  1.00E+20
 cie   2 2 Temperature (keV)      2.9125      1  1.00E-03  1.00E-04  1.00E+03
 cie   3 2 El. dens (1E20/m**3)  1.00000E-04  0  1.00E-03  1.00E-22  1.00E+10
 cie   4 3 Ion temp. (keV)        1.0000      0    0.      1.00E-04  1.00E+07
 cie   5 2 Microturb vel (km/s)       0.      0    0.        0.      3.00E+05
 cie   6 1 Abundance He           1.0000      0  1.00E-03 -1.00E+10  1.00E+10
 cie   7 1 Abundance Li           1.0000      0  1.00E-03 -1.00E+10  1.00E+10
  ..      (shortened)
 cie  34 1 Abundance Zn           1.0000      0  1.00E-03 -1.00E+10  1.00E+10
 absm  1 2 Column (1E28/m**2)    1.22782E-05  1  1.00E-03    0.      1.00E+10
------------------------------------------------------------------------------
 Fluxes and restframe luminosities between  0.20000     and    12.000     keV

  nr mod   photon flux   energy flux nr of photons    luminosity
         (phot/m**2/s)      (W/m**2)   (photons/s)          (W)
   1 cie    100.36      1.73397E-14  1.05685E+39  1.80332E+23
 Chi-squared value :       221.72
 Degrees of freedom:   227
```

Comment: After the fitting procedure is completed, SPEX displays the current values of the spectral model parameters. Notation: `mod` denotes the model components to which a specific parameter belongs. `nr` denotes the parameter number of the model component. `t` is a model specific parameter that defines the type of the parameter. t ranges from 0 to 3. 0 = normalization parameter; 1 = abundance parameter;

2 = fit parameter; 3 = non–fit parameter. `parameter with unit` describes the spectral model parameter and shows the corresponding unit. `value` denotes the current value of the parameter in the specified unit. `st` denotes the status of the parameter. 0 = frozen; 1 = fitable/free. Each parameter may be fitted (if allowed) in the range between `minimum` and `maximum` with stepsize `step`. Finally, fluxes and luminosities are shown for the additive component (CIE).

```
------------------------------------------------------------------------
 mod  nr parameter with unit   mod  nr parameter with unit   correlation

 cie   2 Temperature (keV)     cie   2 Temperature (keV)       1.0000
 cie   2 Temperature (keV)     absm  1 Column (1E28/m**2)    -0.99998
 absm  1 Column (1E28/m**2)    absm  1 Column (1E28/m**2)      1.0000
------------------------------------------------------------------------
 mod  nr parameter with unit   mod  nr parameter with unit   correlation

 cie   1 ne nH V (1E64/m**3)   cie   1 ne nH V (1E64/m**3)     1.0000
 Normal end of input file encountered
```

Comment: Next, SPEX shows the correlations between the free fit parameters (above) and the normalization parameters (below). See Press et al. (1992) for more information about the correlation of fit parameters.

```
------------------------ SPEX Version  1.00 -------------------------
---------------------------- SPEX fit menu ----------------------------
| fit  | Description                                                   |
------------------------------------------------------------------------
| METH | change the spectral fitting method                            |
| RUN  | fit the parameters using current data & model                 |
| ERR  | determine error bounds on parameters                          |
| STEP | do a grid search                                              |
| MAIN | Back to main menu                                             |
------------------------------------------------------------------------
Enter your choice [RUN ]:main
```

Comment: `main` is entered to return to the main menu.

2.7 Plot of observed and fitted data

```
------------------------ SPEX Version  1.00 ------------------------
-------------------------- SPEX main menu --------------------------
| main | Description                                                  |
---------------------------------------------------------------------
| QUIT | Exit from SPEX                                               |
| HIDE | Hide (do not hide) menu listings (for experienced user only) |
| LOG  | Log file: save or read log files for commands and output     |
| DIST | Set the source distance                                      |
| GRID | Select default energy grid                                   |
| ELIM | Set energy limits for flux calculations                      |
| VAR  | Define default abundances and line properties etc.           |
| DATA | Read, write, show or modify data (response & obs. spectrum)  |
| MOD  | Modify the spectral model                                    |
| PAR  | Modify the current model parameters                          |
| CALC | Evaluate the current spectral model                          |
| SIM  | Simulate a spectrum using current model & detector           |
| FIT  | Spectral fitting, error search etc.                          |
| ASC  | Output of SPEX model properties to ascii file or screen      |
| PLOT | Plot menu                                                    |
---------------------------------------------------------------------
Enter your choice [DIST]:plot
```

Comment: `plot` is entered to go to the plot menu to make a plot of the observed and fitted data.

```
------------------------ SPEX Version  1.00 -------------------------
--------------------------- SPEX plot menu ----------------------------
| pmen | Description                                                   |
---------------------------------------------------------------------
| TYPE | Select a new plot type                                        |
| PLOT | Do the plot                                                   |
| DEV  | Set plotting device                                           |
| NAME | Set plot file name                                            |
| HLAN | PostScript print (landscape mode)                             |
| HPOR | PostScript print (portrait mode)                              |
| LX   | Change x-axis scale scale logarithmic / linear                |
| LY   | Change y-axis scale scale logarithmic / linear                |
| UX   | Redefine x-axis units                                         |
| UY   | Redefine y-axis units                                         |
| RX   | Modify x-axis range                                           |
| RY   | Modify y-axis range                                           |
| FONT | Change font type                                              |
| FH   | Change font height                                            |
| CAP  | Modify caption texts                                          |
| SYMB | Change plot symbols                                           |
| HIS  | Histogram / continuous line plot mode                         |
| LW   | Change line weights                                           |
| LT   | Change line styles                                            |
| COL  | Change plot colours                                           |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [PLOT]:dev
```

Comment: `dev` is selected to define the plotting device. Note that the default plotting device at program startup is the null device, i.e. there will be no output.

```
------------------------ SPEX Version  1.00 -------------------------
-------------------------- Set plot device ---------------------------
| pdev | Description                                                   |
---------------------------------------------------------------------
| NULL | Null device, no output                                        |
| PS   | PostScript file, landscape orientation                        |
| VPS  | PostScript file, portrait orientation                         |
| CPS  | Colour PostScript file, landscape orientation                 |
| VCPS | Colour PostScript file, portrait orientation                  |
| XTER | XTERM Tek terminal emulator                                   |
| XWIN | Window on Xwindow server                                      |
| XDIS | Pgdisp or figdisp server                                      |
---------------------------------------------------------------------
Enter your choice [XWIN]:ps
```

Comment: Various plotting devices are available. In this example the plotting device will be a PostScript file with landscape orientation, thus `ps` is entered.

```
------------------------- SPEX Version  1.00 -------------------------
--------------------------- SPEX plot menu ---------------------------
| pmen | Description                                                   |
-------------------------------------------------------------------------
| TYPE | Select a new plot type                                        |
| PLOT | Do the plot                                                   |
| DEV  | Set plotting device                                           |
| NAME | Set plot file name                                            |
| HLAN | PostScript print (landscape mode)                             |
| HPOR | PostScript print (portrait mode)                              |
| LX   | Change x-axis scale scale logarithmic / linear                |
| LY   | Change y-axis scale scale logarithmic / linear                |
| UX   | Redefine x-axis units                                         |
| UY   | Redefine y-axis units                                         |
| RX   | Modify x-axis range                                           |
| RY   | Modify y-axis range                                           |
| FONT | Change font type                                              |
| FH   | Change font height                                            |
| CAP  | Modify caption texts                                          |
| SYMB | Change plot symbols                                           |
| HIS  | Histogram / continuous line plot mode                         |
| LW   | Change line weights                                           |
| LT   | Change line styles                                            |
| COL  | Change plot colours                                           |
| MAIN | Back to main menu                                             |
-------------------------------------------------------------------------
Enter your choice [PLOT]:name

Give plotfile name (with .ps extension) [spex]:iipeg3a.ps
```

Comment: The name of the PostScript file is set by entering `name` and the name of the file `iipeg3a.ps` .

```
------------------------- SPEX Version  1.00 -------------------------
--------------------------- SPEX plot menu ---------------------------
| pmen | Description                                                   |
-----------------------------------------------------------------------
| TYPE | Select a new plot type                                        |
| PLOT | Do the plot                                                   |
| DEV  | Set plotting device                                           |
| NAME | Set plot file name                                            |
| HLAN | PostScript print (landscape mode)                             |
| HPOR | PostScript print (portrait mode)                              |
| LX   | Change x-axis scale scale logarithmic / linear                |
| LY   | Change y-axis scale scale logarithmic / linear                |
| UX   | Redefine x-axis units                                         |
| UY   | Redefine y-axis units                                         |
| RX   | Modify x-axis range                                           |
| RY   | Modify y-axis range                                           |
| FONT | Change font type                                              |
| FH   | Change font height                                            |
| CAP  | Modify caption texts                                          |
| SYMB | Change plot symbols                                           |
| HIS  | Histogram / continuous line plot mode                         |
| LW   | Change line weights                                           |
| LT   | Change line styles                                            |
| COL  | Change plot colours                                           |
| MAIN | Back to main menu                                             |
-----------------------------------------------------------------------
Enter your choice [PLOT]:
```

Comment: The plot may be written to the PostScript file by entering `plot` . The content of this file is displayed in Fig. 2.2.

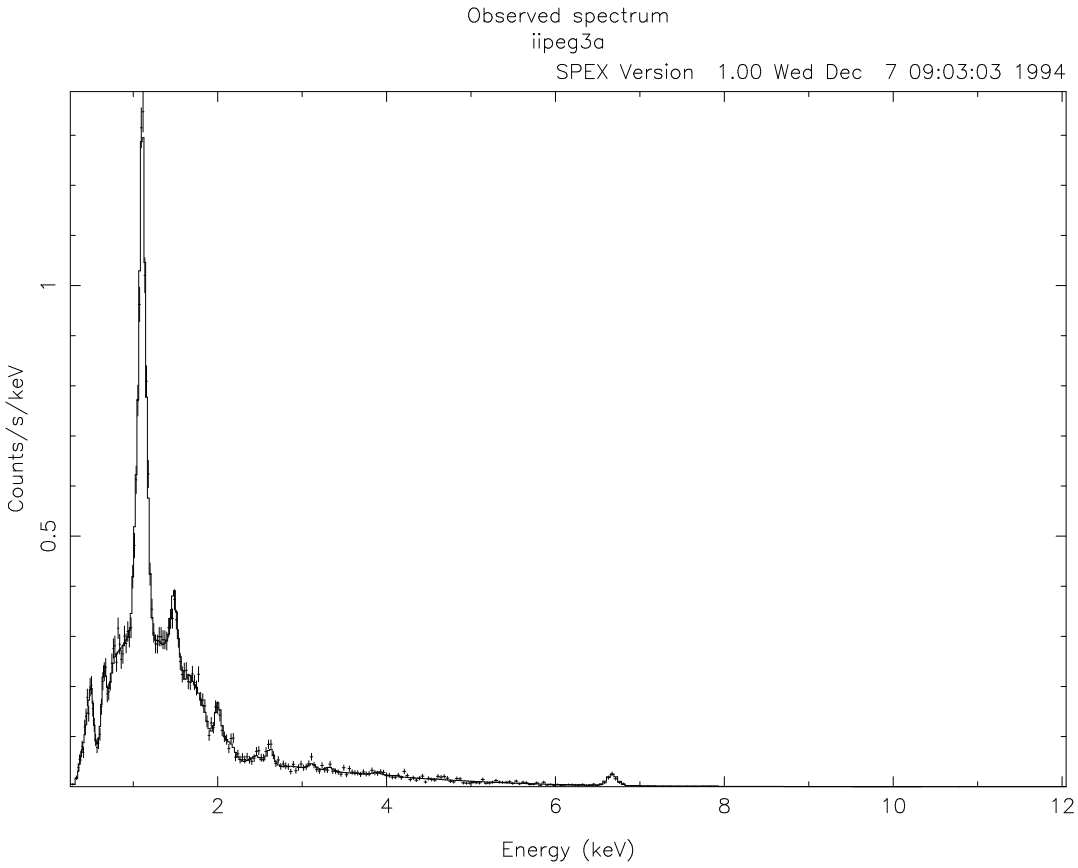

Figure 2.2: The first plot of the observed and fitted data made with SPEX (all settings are the default settings at program startup).

```
------------------------- SPEX Version  1.00 -------------------------
--------------------------- SPEX plot menu ---------------------------
| pmen | Description                                                   |
-----------------------------------------------------------------------
| TYPE | Select a new plot type                                        |
| PLOT | Do the plot                                                   |
| DEV  | Set plotting device                                           |
| NAME | Set plot file name                                            |
| HLAN | PostScript print (landscape mode)                             |
| HPOR | PostScript print (portrait mode)                              |
| LX   | Change x-axis scale scale logarithmic / linear                |
| LY   | Change y-axis scale scale logarithmic / linear                |
| UX   | Redefine x-axis units                                         |
| UY   | Redefine y-axis units                                         |
| RX   | Modify x-axis range                                           |
| RY   | Modify y-axis range                                           |
| FONT | Change font type                                              |
| FH   | Change font height                                            |
| CAP  | Modify caption texts                                          |
| SYMB | Change plot symbols                                           |
| HIS  | Histogram / continuous line plot mode                         |
| LW   | Change line weights                                           |
| LT   | Change line styles                                            |
| COL  | Change plot colours                                           |
| MAIN | Back to main menu                                             |
-----------------------------------------------------------------------
Enter your choice [PLOT]:ux
```

Comment: The plot in Fig. 2.2 was made using the default settings belonging to the default plot type at program startup. `ux` is entered to change the units of the x–axis.

```
------------------------- SPEX Version  1.00 -------------------------
------------------------ Set unit x-axis for data --------------------
| uxda | Description                                                   |
-----------------------------------------------------------------------
| BIN  | Bin nr.                                                       |
| KEV  | Energy (keV)                                                  |
| RYD  | Energy (Rydberg)                                              |
| HZ   | Frequency (Hz)                                                |
| ANG  | Wavelength (A)                                                |
| NM   | Wavelength (nm)                                               |
| M    | Wavelength (m)                                                |
-----------------------------------------------------------------------
Enter your choice [KEV ]:nm
```

Comment: `nm` is entered to set the x–axis units to nm (nanometers).

```
------------------------ SPEX Version  1.00 -------------------------
--------------------------- SPEX plot menu ----------------------------
| pmen | Description                                                   |
---------------------------------------------------------------------
| TYPE | Select a new plot type                                        |
| PLOT | Do the plot                                                   |
| DEV  | Set plotting device                                           |
| NAME | Set plot file name                                            |
| HLAN | PostScript print (landscape mode)                             |
| HPOR | PostScript print (portrait mode)                              |
| LX   | Change x-axis scale scale logarithmic / linear                |
| LY   | Change y-axis scale scale logarithmic / linear                |
| UX   | Redefine x-axis units                                         |
| UY   | Redefine y-axis units                                         |
| RX   | Modify x-axis range                                           |
| RY   | Modify y-axis range                                           |
| FONT | Change font type                                              |
| FH   | Change font height                                            |
| CAP  | Modify caption texts                                          |
| SYMB | Change plot symbols                                           |
| HIS  | Histogram / continuous line plot mode                         |
| LW   | Change line weights                                           |
| LT   | Change line styles                                            |
| COL  | Change plot colours                                           |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [PLOT]:uy
```

Comment: The units of the y–axis will be changed to Counts/s by first entering `uy` .

```
------------------------ SPEX Version  1.00 -------------------------
------------------------ Set unit y-axis for data -------------------
| uyda | Description                                                   |
---------------------------------------------------------------------
| BIN  | Bin nr.                                                       |
| COU  | Counts                                                        |
| CS   | Counts/s                                                      |
| KEV  | Counts/s/keV                                                  |
| RYD  | Counts/s/Ryd                                                  |
| HZ   | Counts/s/Hz                                                   |
| ANG  | Counts/s/A                                                    |
| NM   | Counts/s/nm                                                   |
| M    | Counts/s/m                                                    |
| FCS  | Counts/m**2/s                                                 |
| FKEV | Counts/m**2/s/keV                                             |
| FRYD | Counts/m**2/s/Ryd                                             |
| FHZ  | Counts/m**2/s/Hz                                              |
| FANG | Counts/m**2/s/A                                               |
| FNM  | Counts/m**2/s/nm                                              |
| FM   | Counts/m**2/s/m                                               |
---------------------------------------------------------------------
Enter your choice [KEV ]:cs
```

Comment: `cs` will set the units of the y–axis to Counts per second.

```
------------------------ SPEX Version  1.00 ------------------------
--------------------------- SPEX plot menu ---------------------------
| pmen | Description                                                  |
-------------------------------------------------------------------
| TYPE | Select a new plot type                                       |
| PLOT | Do the plot                                                  |
| DEV  | Set plotting device                                          |
| NAME | Set plot file name                                           |
| HLAN | PostScript print (landscape mode)                            |
| HPOR | PostScript print (portrait mode)                             |
| LX   | Change x-axis scale scale logarithmic / linear               |
| LY   | Change y-axis scale scale logarithmic / linear               |
| UX   | Redefine x-axis units                                        |
| UY   | Redefine y-axis units                                        |
| RX   | Modify x-axis range                                          |
| RY   | Modify y-axis range                                          |
| FONT | Change font type                                             |
| FH   | Change font height                                           |
| CAP  | Modify caption texts                                         |
| SYMB | Change plot symbols                                          |
| HIS  | Histogram / continuous line plot mode                        |
| LW   | Change line weights                                          |
| LT   | Change line styles                                           |
| COL  | Change plot colours                                          |
| MAIN | Back to main menu                                            |
-------------------------------------------------------------------
Enter your choice [PLOT]:
```

Comment: `plot` is entered to generate another PostScript plot, displayed in Fig. 2.3. Note that the PostScript file is not overwritten by this option. The generated PostScript file is appended to the end of the PostScript file, i.e. plotted on a "new" page.

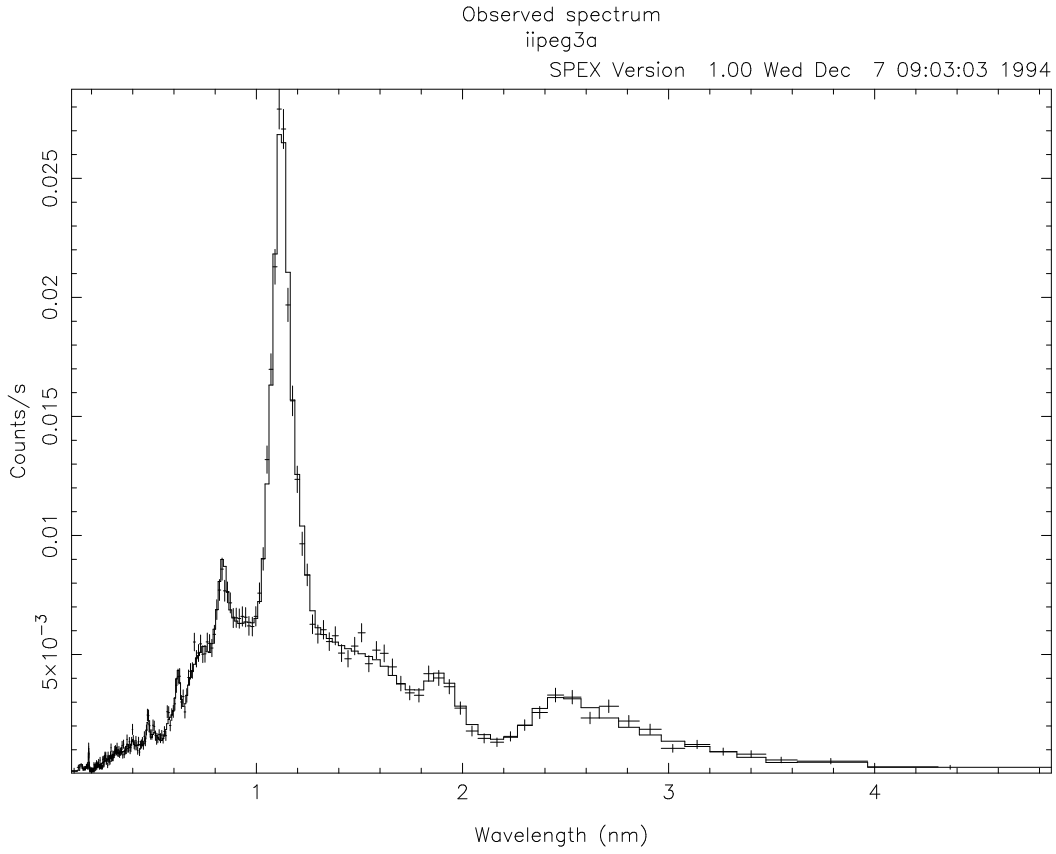

Figure 2.3: Plot of the observed and fitted data in customized units.

```
------------------------- SPEX Version  1.00 -------------------------
--------------------------- SPEX plot menu ---------------------------
| pmen | Description                                                  |
-------------------------------------------------------------------
| TYPE | Select a new plot type                                       |
| PLOT | Do the plot                                                  |
| DEV  | Set plotting device                                          |
| NAME | Set plot file name                                           |
| HLAN | PostScript print (landscape mode)                            |
| HPOR | PostScript print (portrait mode)                             |
| LX   | Change x-axis scale scale logarithmic / linear               |
| LY   | Change y-axis scale scale logarithmic / linear               |
| UX   | Redefine x-axis units                                        |
| UY   | Redefine y-axis units                                        |
| RX   | Modify x-axis range                                          |
| RY   | Modify y-axis range                                          |
| FONT | Change font type                                             |
| FH   | Change font height                                           |
| CAP  | Modify caption texts                                         |
| SYMB | Change plot symbols                                          |
| HIS  | Histogram / continuous line plot mode                        |
| LW   | Change line weights                                          |
| LT   | Change line styles                                           |
| COL  | Change plot colours                                          |
| MAIN | Back to main menu                                            |
-------------------------------------------------------------------
Enter your choice [PLOT]:main
```

Comment: `main` is entered to return to the main menu.

2.8 Accuracy of the fitted parameters

```
------------------------ SPEX Version  1.00 -------------------------
--------------------------- SPEX main menu ----------------------------
| main | Description                                                   |
---------------------------------------------------------------------
| QUIT | Exit from SPEX                                                |
| HIDE | Hide (do not hide) menu listings (for experienced user only)  |
| LOG  | Log file: save or read log files for commands and output       |
| DIST | Set the source distance                                       |
| GRID | Select default energy grid                                    |
| ELIM | Set energy limits for flux calculations                       |
| VAR  | Define default abundances and line properties etc.            |
| DATA | Read, write, show or modify data (response & obs. spectrum)   |
| MOD  | Modify the spectral model                                     |
| PAR  | Modify the current model parameters                           |
| CALC | Evaluate the current spectral model                           |
| SIM  | Simulate a spectrum using current model & detector            |
| FIT  | Spectral fitting, error search etc.                           |
| ASC  | Output of SPEX model properties to ascii file or screen       |
| PLOT | Plot menu                                                     |
---------------------------------------------------------------------
Enter your choice [DIST]:fit
```

Comment: `fit` is entered to go to the fitting menu.

```
------------------------ SPEX Version  1.00 -------------------------
--------------------------- SPEX fit menu -----------------------------
| fit  | Description                                                   |
---------------------------------------------------------------------
| METH | change the spectral fitting method                            |
| RUN  | fit the parameters using current data & model                 |
| ERR  | determine error bounds on parameters                          |
| STEP | do a grid search                                              |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [RUN ]:err
```

Comment: `err` is entered to determine the error bounds on one of the model parameters.

```
------------------------ SPEX Version  1.00 -------------------------
------------------ Search errors of spectral parameters --------------
| err  | Description                                                   |
---------------------------------------------------------------------
| COMP | Select the spectral component for error search                |
| PARA | Select the parameter for the current component                |
| DCHI | Set level of Delta chi**2 for the errors                      |
| RUN  | Determine the errors                                          |
| BACK | Back to previous menu                                         |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [RUN ]:comp
```

Comment: `comp` is entered to select a spectral component.

```
------------------------ SPEX Version  1.00 -------------------------
---------------------- Select a spectral component ------------------
| comp | Description                                                  |
---------------------------------------------------------------------
| A01  | Additive component  1                                        |
| M01  | Multiplicative component  1                                  |
---------------------------------------------------------------------
Enter your choice [A01 ]:m01
```

Comment: `m01` is entered to select the multiplicative component (i.e. ABSM).

```
------------------------ SPEX Version  1.00 -------------------------
------------------ Search errors of spectral parameters --------------
| err  | Description                                                   |
---------------------------------------------------------------------
| COMP | Select the spectral component for error search                |
| PARA | Select the parameter for the current component                |
| DCHI | Set level of Delta chi**2 for the errors                      |
| RUN  | Determine the errors                                          |
| BACK | Back to previous menu                                         |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [RUN ]:para
```

Comment: `para` is entered to select a parameter from the current spectral model component (ABSM).

```
------------------------- SPEX Version  1.00 -------------------------
---------------- Select a spectral parameter (absorption M&M) --------
| sabs | Description                                                   |
-------------------------------------------------------------------
| NH   | Hydrogen column density (1E28 /m**2 = 1E24 /cm**2)            |
-------------------------------------------------------------------
Enter your choice [NH  ]:
```

Comment: The multiplicative ABSM model component only has one parameter. `nh` is entered to select the Hydrogen column density.

```
------------------------- SPEX Version  1.00 -------------------------
------------------ Search errors of spectral parameters --------------
| err  | Description                                                   |
-------------------------------------------------------------------
| COMP | Select the spectral component for error search                |
| PARA | Select the parameter for the current component                |
| DCHI | Set level of Delta chi**2 for the errors                      |
| RUN  | Determine the errors                                          |
| BACK | Back to previous menu                                         |
| MAIN | Back to main menu                                             |
-------------------------------------------------------------------
Enter your choice [RUN ]:
```

Comment: `run` is entered to start the determination of the error bounds of the Hydrogen column density parameter from the ABSM model component.

```
Trial parameter        Chi**2 Delta(parameter) Delta(Chi**2)
  1.21528E-05          221.72  -1.25478E-07            0.00
  1.20273E-05          221.72  -2.50956E-07            0.00
  1.17763E-05          221.72  -5.01911E-07            0.00
  1.12744E-05          221.72  -1.00382E-06            0.00
  1.02706E-05          221.72  -2.00765E-06            0.00
  8.26294E-06          221.74  -4.01529E-06            0.02
  4.24765E-06          221.80  -8.03058E-06            0.08
       0.              221.90  -1.22782E-05            0.18
  1.24037E-05          221.72   1.25478E-07            0.00
  1.25292E-05          221.72   2.50956E-07            0.00
  1.27801E-05          221.72   5.01911E-07            0.00
  1.32821E-05          221.72   1.00382E-06            0.00
  1.42859E-05          221.73   2.00765E-06            0.01
  1.62935E-05          221.74   4.01529E-06            0.02
  2.03088E-05          221.81   8.03058E-06            0.09
  2.83394E-05          222.06   1.60612E-05            0.34
  4.44006E-05          223.03   3.21223E-05            1.31
  7.65229E-05          226.75   6.42447E-05            5.03
  4.44006E-05          223.03   3.21223E-05            1.31
  5.03866E-05          223.54   3.81083E-05            1.82
  5.23236E-05          223.73   4.00454E-05            2.01
Parameter:   1.22782E-05 Errors:  -1.22782E-05,  4.00454E-05
```

Comment: SPEX displays a trial paramtere, the χ^2 value, the difference between the trial value and the current value of the parameter and the $\Delta\chi^2$.

```
------------------------ SPEX Version  1.00 -------------------------
------------------ Search errors of spectral parameters --------------
| err  | Description                                                   |
---------------------------------------------------------------------
| COMP | Select the spectral component for error search                |
| PARA | Select the parameter for the current component                |
| DCHI | Set level of Delta chi**2 for the errors                      |
| RUN  | Determine the errors                                          |
| BACK | Back to previous menu                                         |
| MAIN | Back to main menu                                             |
---------------------------------------------------------------------
Enter your choice [RUN ]:main
```

Comment: `main` is entered to return to the main menu.

```
------------------------- SPEX Version  1.00 -------------------------
--------------------------- SPEX main menu ---------------------------
| main | Description                                                   |
-----------------------------------------------------------------------
| QUIT | Exit from SPEX                                                |
| HIDE | Hide (do not hide) menu listings (for experienced user only)  |
| LOG  | Log file: save or read log files for commands and output       |
| DIST | Set the source distance                                       |
| GRID | Select default energy grid                                    |
| ELIM | Set energy limits for flux calculations                       |
| VAR  | Define default abundances and line properties etc.            |
| DATA | Read, write, show or modify data (response & obs. spectrum)   |
| MOD  | Modify the spectral model                                     |
| PAR  | Modify the current model parameters                           |
| CALC | Evaluate the current spectral model                           |
| SIM  | Simulate a spectrum using current model & detector            |
| FIT  | Spectral fitting, error search etc.                           |
| ASC  | Output of SPEX model properties to ascii file or screen       |
| PLOT | Plot menu                                                     |
-----------------------------------------------------------------------
Enter your choice [FIT ]:plot
```

Comment: The last step in this example will be to make a plot of the fit residuals. Therefore `plot` is entered.

```
------------------------ SPEX Version  1.00 ------------------------
 --------------------------- SPEX plot menu ----------------------------
 | pmen | Description                                                   |
 ---------------------------------------------------------------------
 | TYPE | Select a new plot type                                        |
 | PLOT | Do the plot                                                   |
 | DEV  | Set plotting device                                           |
 | NAME | Set plot file name                                            |
 | HLAN | PostScript print (landscape mode)                             |
 | HPOR | PostScript print (portrait mode)                              |
 | LX   | Change x-axis scale scale logarithmic / linear                |
 | LY   | Change y-axis scale scale logarithmic / linear                |
 | UX   | Redefine x-axis units                                         |
 | UY   | Redefine y-axis units                                         |
 | RX   | Modify x-axis range                                           |
 | RY   | Modify y-axis range                                           |
 | FONT | Change font type                                              |
 | FH   | Change font height                                            |
 | CAP  | Modify caption texts                                          |
 | SYMB | Change plot symbols                                           |
 | HIS  | Histogram / continuous line plot mode                         |
 | LW   | Change line weights                                           |
 | LT   | Change line styles                                            |
 | COL  | Change plot colours                                           |
 | MAIN | Back to main menu                                             |
 ---------------------------------------------------------------------
 Enter your choice [PLOT]:type
```

Comment: In the plot menu, `type` is entered to select a new plot type.

```
------------------------ SPEX Version  1.00 ------------------------
 ------------------------- Select the plot type ---------------------
 | ptyp | Description                                                  |
 ---------------------------------------------------------------------
 | COMP | Select a plasma component for plotting                       |
 | DATA | Observed spectrum & predicted model                          |
 | MOD  | Model photon spectrum                                        |
 | AREA | Effective area of the detector                               |
 | RESP | Response matrix                                              |
 | CHI2 | Fit residuals                                                |
 | SPEC | Plasma model: Continuum and line emission components         |
 | MAIN | Back to main menu                                            |
 ---------------------------------------------------------------------
 Enter your choice [DATA]:chi2
```

Comment: `chi2` is entered to change the plot type to "fit residuals".

```
------------------------- SPEX Version  1.00 -------------------------
--------------------------- SPEX plot menu ---------------------------
| pmen | Description                                                   |
-------------------------------------------------------------------------
| TYPE | Select a new plot type                                        |
| PLOT | Do the plot                                                   |
| DEV  | Set plotting device                                           |
| NAME | Set plot file name                                            |
| HLAN | PostScript print (landscape mode)                             |
| HPOR | PostScript print (portrait mode)                              |
| LX   | Change x-axis scale scale logarithmic / linear                |
| LY   | Change y-axis scale scale logarithmic / linear                |
| UX   | Redefine x-axis units                                         |
| UY   | Redefine y-axis units                                         |
| RX   | Modify x-axis range                                           |
| RY   | Modify y-axis range                                           |
| FONT | Change font type                                              |
| FH   | Change font height                                            |
| CAP  | Modify caption texts                                          |
| SYMB | Change plot symbols                                           |
| HIS  | Histogram / continuous line plot mode                         |
| LW   | Change line weights                                           |
| LT   | Change line styles                                            |
| COL  | Change plot colours                                           |
| MAIN | Back to main menu                                             |
-------------------------------------------------------------------------
Enter your choice [PLOT]:
```

Comment: `plot` is entered to make the plot. Since the plot device has not been changed, this plot will be appended to the existing PostScript file. The content of this plot is displayed in Fig. 2.4.

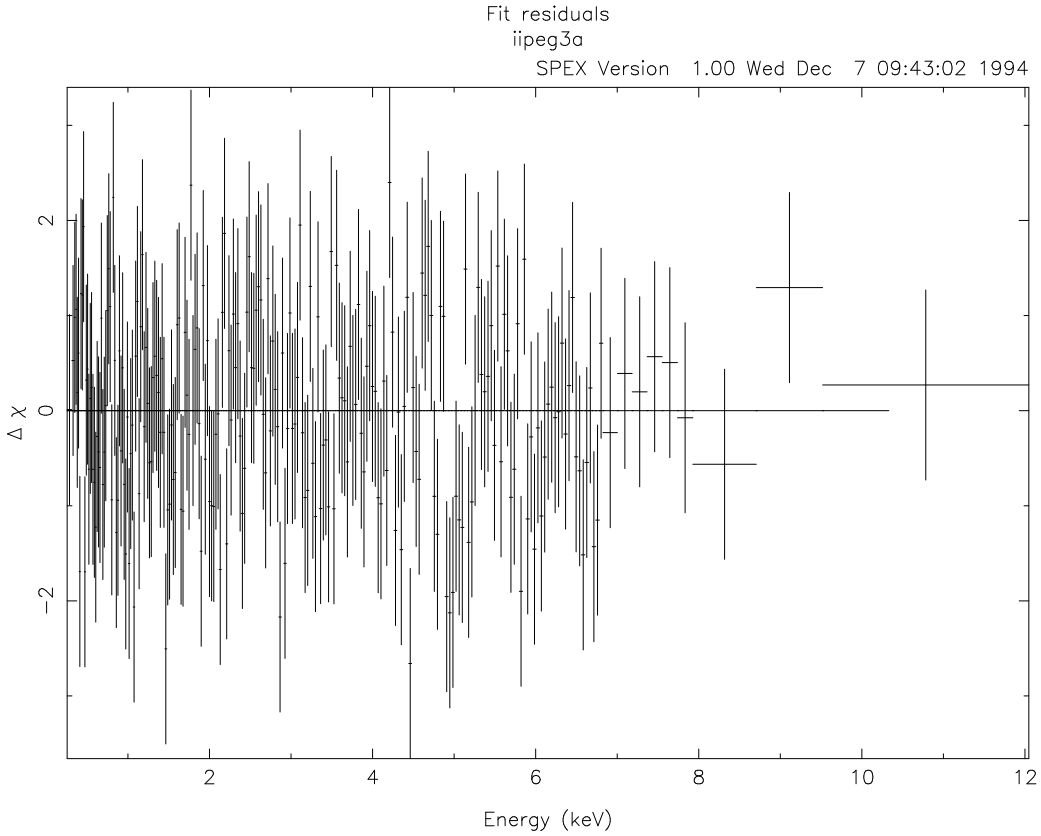

Figure 2.4: Plot of the fit residuals.

```
------------------------- SPEX Version  1.00 -------------------------
--------------------------- SPEX plot menu ---------------------------
| pmen | Description                                                   |
-------------------------------------------------------------------------
| TYPE | Select a new plot type                                        |
| PLOT | Do the plot                                                   |
| DEV  | Set plotting device                                           |
| NAME | Set plot file name                                            |
| HLAN | PostScript print (landscape mode)                             |
| HPOR | PostScript print (portrait mode)                              |
| LX   | Change x-axis scale scale logarithmic / linear                |
| LY   | Change y-axis scale scale logarithmic / linear                |
| UX   | Redefine x-axis units                                         |
| UY   | Redefine y-axis units                                         |
| RX   | Modify x-axis range                                           |
| RY   | Modify y-axis range                                           |
| FONT | Change font type                                              |
| FH   | Change font height                                            |
| CAP  | Modify caption texts                                          |
| SYMB | Change plot symbols                                           |
| HIS  | Histogram / continuous line plot mode                         |
| LW   | Change line weights                                           |
| LT   | Change line styles                                            |
| COL  | Change plot colours                                           |
| MAIN | Back to main menu                                             |
-------------------------------------------------------------------------
 Enter your choice [PLOT]:main
```

Comment: `main` is entered to return to the main menu.

```
------------------------- SPEX Version  1.00 -------------------------
--------------------------- SPEX main menu ---------------------------
| main | Description                                                   |
-------------------------------------------------------------------------
| QUIT | Exit from SPEX                                                |
| HIDE | Hide (do not hide) menu listings (for experienced user only)  |
| LOG  | Log file: save or read log files for commands and output      |
| DIST | Set the source distance                                       |
| GRID | Select default energy grid                                    |
| ELIM | Set energy limits for flux calculations                       |
| VAR  | Define default abundances and line properties etc.            |
| DATA | Read, write, show or modify data (response & obs. spectrum)   |
| MOD  | Modify the spectral model                                     |
| PAR  | Modify the current model parameters                           |
| CALC | Evaluate the current spectral model                           |
| SIM  | Simulate a spectrum using current model & detector            |
| FIT  | Spectral fitting, error search etc.                           |
| ASC  | Output of SPEX model properties to ascii file or screen       |
| PLOT | Plot menu                                                     |
-------------------------------------------------------------------------
Enter your choice [FIT ]:quit
```

Comment: `quit` is entered to exit the SPEX program.

```
------------------------------------------------------------------------
------------------------------------------------------------------------
Normal end of SPEX
Run time statistics (s)
-----------------------

nr. name           elapsed          cpu
---------------------------------------
301 setabu              0.20         0.03
311 slinsort            0.73         0.03
401 layerstart          0.01         0.01
402 ciescale            0.02         0.02
405 addspec            12.37         0.31
406 layerend            0.02         0.00
501 setcon              0.10         0.03
508 eleion              9.56         0.09
509 ionis2              0.52         0.00
510 augdis              4.31         0.06
511 cheion              0.07         0.01
512 cherec              0.20         0.01
513 recomb              2.03         0.06
514 cestart             0.32         0.00
515 ionrec3             0.24         0.02
516 ioncon              2.24         0.04
517 elhden              0.14         0.05
518 cedec               0.07         0.02
522 gauntff            73.18         0.51
534 brems              43.10         0.24
535 freebound         870.66         5.14
536 twofot              5.52         0.10
537 conem               1.07         0.04
540 linem              29.89         0.39
541 linsort            14.06         0.14
543 linspe             45.14        14.99
544 totspec             0.53         0.00
    SPEX total       1116.30        22.34
---------------------------------------
```

Comment: At the end of the program, SPEX shows for each routine how much processing time it used. (In some implementations of SPEX, this option may not yet function. However, it does work on a SUN workstation). SPEX will also show the number of errors that occured during the input of the commands.

2.9 Using a log file

SPEX provides an option to 'record' and 'play back' SPEX commands using so–called *log files*. These log files are especially useful to be used as 'macros' to do 'routine' jobs such as setting models, reading data etc. A log file is an ASCII file and may be edited with any ASCII editor. In this way, useful sets of SPEX commands may be 'precompiled'. For more information about the SPEX log file strucure, see chapter 7.

All SPEX commands used to generate the example SPEX session in the previous sections are recorded in the file `iipegfit3a.com`. The contents of the log file are displayed below.

```
################################################################
# Title  : SRON/SPEX/TRUM example log file
# File   : iipegfit3a.com
# Date   : September 12, 1994
# Author : F. van der Wolf
# Purpose: This is a log file for the example SPEX
#          session in doc. SRON/SPEX/TRUM. A
#          spectral model (CIE,ABSM will be defined
#          and fitted on a simulated spectrum of II Peg,
#          based on the ASCA-SIS instrument.
################################################################
#
# Define the distance of the source at 29.4 pc
#
disu PC
dist DIST 29.4
# Set the energy limits for the flux calculations
#
elim LOW .2
elim UPP 12.
#
# Read the energy grid from the response matrix: iipeg3a.res
#
gdat NAME iipeg3a
gdat READ
# Read the (previously simulated) spectrum of II Peg
#
read RNAM iipeg3a
read SNAM iipeg3a
read READ
dat  SHOW
#
# Define an additiYe model component: Collisional
#  Equilibrium component (CIE)
#
moda CIE
#
# Define a multiplicative model component: Absorption
#   component (Morrison & McCammon) (ABSM)
#
modb ABSM
#
# Set the relation betueen the additive and multiplicative
# component to 1
```

```
#
mode SAME 1
#
# Show the spectral model
mod SHOW
#
# Modify the spectral model parameters for the CIE
# component (additive)
#
par COMP
comp AO1
#
# Set Normalisation to 1E-5 i.e. 1OE59/m**3
#
par PARA
scie NORM
par VAL 1.E-05
#
# Set Electron Temperature to 3 keV
#
par PARA
scie T
par VAL 3.
#
# Set Ion Temperature to 1 keV
#
par PARA
scie IT
par VAL 1.
#
# Set Electron density to 1E-4 i.e. 1OE16/m**3
#
par PARA
scie ED
par VAl 1.E-04
#
# Set Micro turbulence velocity to O km/s
#
par PARA
scie VMIC
par VAL .E+OO
#
# Modify the spectral model parameters for the ABSM
# component (multiplicative)
#
par COMP
comp MO1
#
```

```
# Set the Hydrogen column density to 5E-6 i.e. 5E18/cm**2
#
par VAL 5.E-06
#
Fit the defined model to the spectrum
fit RUN
#
# Select a PostScript plotting device (Landscape orientation)
#
pdev PS
#
# Name the PostScript file iipeg3a.ps
#
pmen NAME iipeg3a.ps
#
# Write a plot to the PostScript file
pmen PLOT
#
# Change X axis units to nanometers
#
uxda NM
#
# Change Y axis units to Count/second
#
uyda CS
#
# Write another plot to the PostScript file
#
pmen PLOT
#
# Select a model component to determine an error
# bound for one of lts parameters. In this example
# the multiplicative component is chosen...
#
err COMP
comp MO1
#
# ... and the Hydrogen column density is selected
#
par PARA
sabs NH
#
# And the error bounds are determined
#
err RUN
#
# Finally, a plot of the fit residuals is written
# to the PostScript file
```

```
#
ptyp CHI2
pmen PLOT
#
############################################################
```

Chapter 3

SPEX Menu Structure

3.1 Introduction

This chapter presents the complete menu structure of SPEX. To recapitulate: the example SPEX session in Chapter 2 showed more menu options as more data were loaded into SPEX and models were defined. The complete SPEX main menu is displayed in Fig. 3.1. The main menu is displayed in Fig. 3.2 again, now divided into categories of special purposes. The following sections will describe all menu options in each category.

It should be noted that there is no difference in the menu structure for the windows version or the terminal version of SPEX. However, the windows version of SPEX does not use the options **BACK** and **MAIN**, since under windows one uses the mouse to change to different menus.

```
------------------------- SPEX Version  1.00 -------------------------
--------------------------- SPEX main menu ---------------------------
| main | Description                                                  |
-----------------------------------------------------------------------
| QUIT | Exit from SPEX                                               |
| HIDE | Hide (do not hide) menu listings (for experienced user only) |
| LOG  | Log file: save or read log files for commands and output     |
| DIST | Set the source distance                                      |
| GRID | Select default energy grid                                   |
| ELIM | Set energy limits for flux calculations                      |
| VAR  | Define default abundances and line properties etc.           |
| DATA | Read, write, show or modify data (response & obs. spectrum)  |
| MOD  | Modify the spectral model                                    |
| PAR  | Modify the current model parameters                          |
| CALC | Evaluate the current spectral model                          |
| SIM  | Simulate a spectrum using current model & detector           |
| FIT  | Spectral fitting, error search etc.                          |
| DEM  | Differential Emission Measure analysis (DEM)                 |
| ASC  | Output of SPEX model properties to ascii file or screen      |
| PLOT | Plot menu                                                    |
-----------------------------------------------------------------------
```

Figure 3.1: SPEX main menu (terminal mode), once all necessary parameters are loaded into the program.

Figure 3.3 shows the structure in which all menu options are displayed. The main menu consists of two options: M1 and M2. Main menu option M1 (the default at program startup) is titled *m1* and has two sub menu options: S1 and S2 (default). Submenu option S1 — titled *sm1* — represents a new (sub-sub) menu with two options: S11 (default) — titled *ssm1* — and S12, titled *ssm2*. The sub-sub-sub menu options of S1 and S2 are called s111, s112 and S121, S122 respectively. All

menu titles and item names are listed in the index at the end of this manual. These index entries may be used for quick references when new log files are to be created or when old log files must be understood. Besides the default menu options at program startup, the menu structure also shows the default settings (at program startup) for certain parameters or file names.

3.2 Program control

The main menu options in this category control the way SPEX is run.

QUIT Exit from SPEX

When SPEX is run in window mode, this option is not available and SPEX may be left by quitting the main window. In both interactive and window modes all open files are closed and run time statistics are shown.

HIDE Hide/show menu listings (for experienced users only)

This main menu option is a switch to hide or show the menu options. Novice users are advised **not** to use the option to hide the menu listings until they have gained enough experience with SPEX. When SPEX is run in window mode, this option is not available.

When the menu options are hidden, typing `?` at the SPEX prompt will result in the display of the menu options for that particular menu.

LOG Save or read log files for commands and output *log*

SPEX has the option to store and read commands from log files. A log file is a copy of a sequence of commands from a previous SPEX run. It is also possible to store SPEX output into a file. If in the following options no path is specified, SPEX will read or write to a file in the directory from which SPEX was started.

Chapter 7 gives a detailed description of the log file structure and usage of it.

`COM` Set log file for storing your commands *com*

Store commands into a log file. The log file may be used to 'record' steps that can be 'played back' at a later time. After the log file is closed, it may be edited with an ASCII editor, for example to add comment lines (comment lines start with an `#` as the first character of a new line and should be no longer than 256 characters), or to add or delete commands.

Unless the file name is changed, SPEX will use the default file name at program startup (`spex`) or the last defined filename.

NAME Change file name for saving your commands (without .com)

OPEN Open the file for saving your commands

CLOS Close the file for saving your commands

Program control

`QUIT` : Exit from SPEX
`HIDE` : Hide/show menu listings (for experienced user only)
`LOG` : Save or read log files for commands and output

Source parameters & instrumental settings

`DIST` : Set the source distance
`GRID` : Select default energy grid
`ELIM` : Set energy limits for flux calculations
`VAR` : Define default abundances and line properties etc.
`DATA` : Read, write, show or modify data

Spectral model

`MOD` : Modify the spectral model
`PAR` : Modify the current model parameters

Evaluation

`CALC` : Evaluate the current spectral model

Simulation

`SIM` : Simulate a spectrum using current model & detector

Fitting

`FIT` : Fit the parameters using current data & model
`DEM` : Differential emission measure analysis (DEM)

Plots & ASCII files

`ASC` : Output of SPEX model properties to file or screen
`PLOT` : Plot menu

Figure 3.2: SPEX main menu divided into categories.

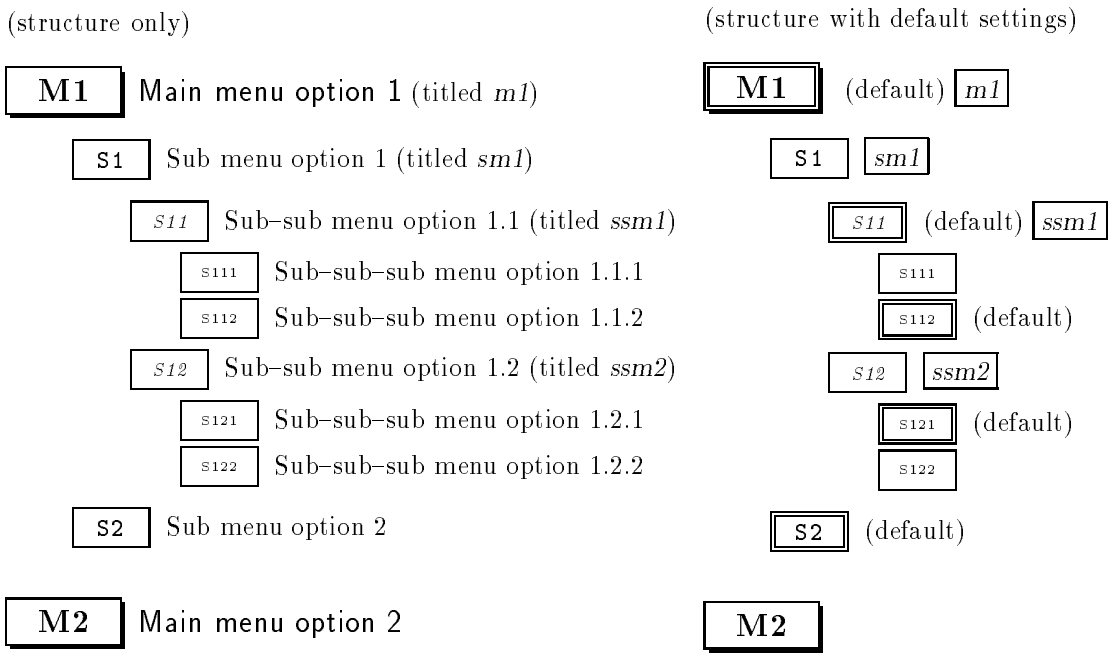

Figure 3.3: Representation of the menu structure. Both trees represent the same structure. The right tree shows the menu titles in a *box* and default options (double boxed) at program startup. Menu titles and item names are listed in the index at the end of this manual.

BACK Back to previous menu

MAIN Back to main menu

EXE Set log file for reading your commands *exe*

Unless the file name is changed, SPEX will use the default file name at program startup (`spex`) or the last defined filename.

NAME Change file name for reading your commands (without .com)

OPEN Open the file for reading your commands

BACK Back to previous menu

MAIN Back to main menu

OUT Set log file for storing SPEX output *out*

Various types of output from SPEX may be stored into a file. At program start all SPEX output will be stored if this option is selected.

Unless the file name is changed, SPEX will use the default file name at program startup (`spex`) or the last defined filename.

PROG Save runtime output (on/off)

SHOW Save data, model and parameter information (on/off)

MENU Save selected menus and items (on/off)

NAME Change file name for SPEX output (without .out)

OPEN Open the file for saving SPEX output

CLOS Close the file for saving SPEX output

BACK Back to previous menu

MAIN Back to main menu

3.3 Source parameters & instrumental settings

The main menu options in this category enable the control of important source specific information such as distance of the source and the abundances of elements. It may also be used to provide SPEX with the necessary data such as energy grids and response matrices of space based instruments.

DIST Set the source distance *dist*

It is very important to set the source at the right distance when additive and multiplicative model components are to be used. SPEX specifically works with luminosities and **not** with fluxes, except of course for the observed and simulated spectra.

UNIT Define the unit of your distance scale *disu*

Internally, SPEX uses a unit of 10^{22} m to prevent machine overflow. Other distance scales internally use their numbers.

SPEX Distance in 10^{22} m

AU Distance in Astronomical units

LY Distance in light years

PC Distance in pc

KPC Distance in kpc

MPC Distance in Mpc

Z Cosmological redshift (use $H_0 = 50$, q_0=0.5)

BACK Back to previous menu

MAIN Back to main menu

DIST Enter the value of the distance in your selected units

Default at program startup is: 1, in SPEX units of 10^{22} m.

`SHOW` Show the current distance and unit

`MAIN` Back to main menu

GRID Select default energy grid *grid*

This menu option sets the default energy grid on which the future calculations will be done. Linear and logarithmical grids may be defined manually. Predefined grids and response matrices of space based instruments may be read from file. The current energy grid may be saved to a file for later use.

The default energy grid at program startup is a logarithmic grid from 10^{-3} – 100 keV, with 8192 steps.

An energy grid **must** be defined before reading in any spectral data. If the default grid is used, interpolations to that grid will be made.

If data is to be appended to an existing data set, the energy grid **must** be redefined in order to cover the full energy range and resolution of both instruments. Otherwise the model is only calculated on the energy grid of the first data set.

If a model contains a red–shift component, the energy grid must be wide enough to cover the spectrum in the source's rest-frame. SPEX calculates the spectrum in the rest frame and then shifts all photons to the observers frame.

The energy grid should defined to be monotonically increasing in energy. If an energy grid is calculated from an increasing wavelength grid, the order of the wavelength grid **must** be reversed to obtain monotonically increasing values of the energy.

`LIN` Linear energy grid *glin*

The energy grid is defined by the lower and upper energy limits, and either the step size or the number of energy bins.

- *LOW* Set lower energy limit (keV)
- *UPP* Set upper energy limit (keV)
- *STEP* Set step size (keV)
- *N* Set number of bins
- *CRE* Make the energy grid
- *BACK* Back to previous menu
- *MAIN* Back to main menu

`LOG` Logarithmic energy grid *glog*

The energy grid is defined by the lower and upper energy limits, and either the step size or the number of energy bins.

- *LOW* Set lower energy limit (keV)
- *UPP* Set upper energy limit (keV)
- *STEP* Set log step size (keV)
- *N* Set number of bins
- *CRE* Make the energy grid
- *BACK* Back to previous menu
- *MAIN* Back to main menu

FILE Input an energy grid from a file *gfil*

Unless the file name is changed, SPEX will use the default file name at program startup (**spex**) or the last defined filename.

- *NAME* Change file name of file with energy grid
- *READ* Read the file with the energy grid
- *BACK* Back to previous menu
- *MAIN* Back to main menu

DATA Input the grid of a response matrix *gdat*

Unless the file name is changed, SPEX will use the default file name at program startup (**spex**) or the last defined filename.

- *NAME* Change file name of response matrix with energy grid
- *READ* Read the file with the energy grid
- *BACK* Back to previous menu
- *MAIN* Back to main menu

SAVE Save the current energy grid to a file *gsav*

Unless the file name is changed, SPEX will use the default file name at program startup (**spex**) or the last defined filename.

- *NAME* Change file name of file for energy grid
- *SAVE* Save the energy grid to the file
- *BACK* Back to previous menu
- *MAIN* Back to main menu

MAIN Back to main menu

ELIM Set the energy limits for flux calculations *elim*

It is possible to define an energy range for which fluxes and luminosities are calculated each time SPEX evaluates the current spectral model. The default energy range at program startup is 2 – 10 keV.

- LOW Set lower energy limit (keV)
- UPP Set upper energy limit (keV)
- MAIN Back to main menu

VAR Define default abundances and line properties etc. *var*

Several basic settings of the plasma models may be adjusted.

 Novice users are discouraged to change the settings until they have gained enough experience with SPEX.

ABUN Set the standard set of abundances *abun*

In SPEX the plasma emission is calculated using element abundances expressed in specified standard units. The default abundance set is that of Anders & Grevesse (1989), which are solar photospheric values. The available options are displayed below, however in most cases the Anders & Grevesse (1989) set is recommended.

- *STAN* Solar abundances (Anders & Grevesse 1989)
- *ALL* Solar abundances (Allen 1973)
- *ROSS* Solar abundances (Ross & Aller 1976)
- *GREV* Solar abundances (Grevesse 1992)
- *BACK* Back to previous menu
- *MAIN* Back to main menu

IBAL Ionisation balance for CIE-plasmas *ibal*

SPEX offers the opportunity to change the ionisation balance for CIE-plasmas. The default (and recommended) set of ionisation and recombination rates is currently Arnaud & Raymond (1992) for iron and Arnaud & Rothenflug (1985) for the other elements.

 For NEI-spectra, like e.g. the supernova remnant models, *always* the default rates are used.

- *DEF* Use SPEX default (currently Arnaud & Raymond for Fe)
- *85* Arnaud & Rothenflug 1985
- *92* Arnaud & Rothenflug 1985 + Arnaud & Raymond 1992 for Fe

BACK Back to previous menu

MAIN Back to main menu

GACC Set accuracy for free-bound Gaunt factor *gacc*

The free-bound gaunt factors as calculated by SPEX have limited accuracy. Contributions from ions with low abundances or from the highest excited levels of other ions to the total effective gaunt factor are usually small. SPEX uses this by neglecting contributions from energy levels from ions that contribute less than a relative factor $\sim g_{\rm acc}$ to the total free-bound Gaunt factor. Default value is $g_{\rm acc} = 10^{-3}$. The user may change this level (for very accurate calculations, or alternatively for very fast rough calculations). Note however that computation time increases very rapidly with increasing accuracy level! The current default represents a fair compromise between computational speed and accuracy.

DEF Use default value (1E-3 for solar abundances)

SET Set your own accuracy

BACK Back to previous menu

MAIN Back to main menu

LINE Change line emission properties *line*

To investigate the influence of specific plasma emission processes, SPEX offers the possibility to switch them on or off. This is for testing purposes only, make sure that all options are set when calculating realistic spectra.

EX Include (not) collisional excitation

RR Include (not) radiative recombination

DR Include (not) dielectronic recombination (main line)

DS Include (not) dielectronic recombination satellites

II Include (not) inner shell ionisation

COMB Combine (not) all line contributions into single line

BACK Back to previous menu

MAIN Back to main menu

DOPP Select line broadening mechanism *ld*

The ion temperature and micro turbulence can be set by changing the spectral model parameters.

NO No line broadening

DOPP Thermal Doppler broadening by ions and microturbulence

BACK Back to previous menu

MAIN Back to main menu

LCAL Set type of line calculation (old or new) *lcal*

This offers the opportunity to choose between the old "mekal" model, and the newer "spex" calculations, that become gradually available for more ions.

OLD Use old plasma code (mekal)

NEW Use new plasma code (spex)

BACK Back to previous menu

MAIN Back to main menu

MAIN Back to main menu

DATA Read, write, show or modify data (response & obs. spectrum) *dat*

This is the file I/O option for data of the SPEX program. Spectral data and response files may be read and/or written. Data sets may be modified.


To learn more about the various file formats, see chapter 6.

FORM Set the format of the data files (binary or ascii) *form*

BIN Set the format of the data files to binary mode

ASC Set the format of the data files to ascii mode

BACK Back to previous menu

TYPE Type of data to be read or written (res, spo or res & spo) *dtyp*

RES Response file to be read or written

SPO Spectra file to be read or written

ALL Both spectra and response files to be read or written

BACK Back to previous menu

COMB How are the new data to be combined with the old data *comb*

NEW Read a new data set

Any existing data set in SPEX's memory will be overwritten with the newly selected data set.

PLUS Read a new data set & add per channel to old data

The new and old data set must have the same energy grid and number of channels. This option is useful for combining spectra obtained simultaneously by two (nearly) identical detectors, e.g. the two ASCA SIS detectors.

MEAN Read a new data set & average with old data set

The new and old data set must have the same energy grid and number of channels. This option is useful for combining e.g. spectra taken at different epochs with the same instrument for an analysis of the time averaged spectrum. Example: two SIS spectra of Cas A, obtained by ASCA at different dates.

APP Read a new data set & append it after the old data

This option should be used to combine data obtained by two (or more) completely different instruments. The new data channels will be appended after the old channels, thus creating a single combined spectrum and response matrix. Example: combining the SIS and GIS data of ASCA.

BACK Back to previous menu

READ Read new data set (be sure FORM, TYPE and COMB are correct) *read*

Unless the file name is changed, SPEX will use the default file name at program startup (`spex`) or the last defined filename.

RNAM Change file name containing the response matrix

SNAM Change file name containing the spectrum

READ Read the data set from named file

BACK Back to previous menu

MAIN Back to main menu

WRIT Save the current data set (be sure FORM & TYPE are correct) *writ*

Unless the file name is changed, SPEX will use the default file name at program startup (`spex`) or the last defined filename.

RNAM Change file name containing the response matrix

SNAM Change file name containing the spectrum

SAVE Save the data set to named file

BACK Back to previous menu

MAIN Back to main menu

DMOD Modify, rebin or optimise the current data set *dmod*

DEL Delete specified data channels *del*

For example badly calibrated channels, or channels that do not have sufficient flux information can be deleted. If only a certain part of the spectrum should be fitted, this option can also be used. The channels will be deleted from both the spectrum and the response matrix.

After deleting certain channels, all channels above the deleted range have different channel numbers! Therefore if more ranges are to be deleted, one is strongly advised to delete the highest channels first.

One can choose to delete either channel ranges or energy ranges. When channels are deleted by energy, the energy centroid of the channel determines if a channel will be deleted or not.

CE Delete by channel or energy

Switch between deletion of channel ranges or energy ranges.

Default at program startup is: channel.

LOW Specify lower limit delete range

Default at program startup is: data channel 1.

UPP Specify upper limit delete range

Default at program startup is: maximum available data channel in data set.

SEL Add data between lower and upper range to delete selection

DEL Delete the selected range(s)

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EBIN Rebin specific data channels *ebin*

Especially in situations with low statistics per channel (e.g. less than 10 counts per channel), it is advised to rebin the data set in order to create channels with sufficient statistics.

After rebinning specific channels, all channels above the rebinned range have different channel numbers! Therefore if more ranges are to be rebinned, one is strongly advised to rebin the highest channels first.

The number of channels that are to be rebinned should be a multiple of the number of channels that are to be taken together. Example: the lower channel limit is 100, and the upper is 199; the number of channels to be taken together is 25. After rebinning there will be 4 bins, each containing 25 original channels. If the upper channel limit would have been 201, rebinning would result into 4 bins containing 25 original channels and one last bin containing 2 original channels.

LOW Specify lower limit rebin range

Default at program startup is: data channel 1.

UPP Specify upper limit rebin range

Default at program startup is: maximum available data channel in data set.

N Specify number of bins to be taken together

Default at program startup is: 2 bins.

REB Rebin the selected channel range

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VBIN Rebin using minimal bin width & sufficient S/N ratio *vbin*

Especially in situations with low statistics per channel (e.g. less than 10 counts per channel), it is advised to rebin the data set in order to create channels with sufficient statistics. The most significant difference with *EBIN* is that this option generates bins with variable widths, however with a minimum signal to noise ratio. This option is useful for example for high-resolution spectra with strong line emission and very weak continuum.

After rebinning specific channels, all channels above the rebinned range have different channel numbers! Therefore if more ranges are to be rebinned, one is strongly advised to rebin the highest channels first.

It is not always guaranteed that the minimum signal-to-noise ratio is obtained in all channels. This is an effect of the applied algorithm. Channels with the highest S/N ratio and neighbouring bins are merged until sufficient S/N ratio is obtained. This process is continued for the remaining number of bins. At the end of the process a few bins with a low S/N ratio will remain. These are merged with their neighbours, resulting in a possibly lower S/N ratio for that bin.

LOW Specify lower limit rebin range

Default at program startup is: data channel 1.

UPP Specify upper limit rebin range

Default at program startup is: maximum available data channel in data set.

N Specify mimimum number of bins to be taken together

Default at program startup is: 2 bins.

SN Specify mimimum signal-to-noise ratio per bin

Default at program startup is: 3.

REB Rebin the selected channel range

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MUL Multiply the response by a constant

This option is useful in two situations. One when spectral data from two instruments are to be combined and there is uncertainty in the absolute calibration of one of the instruments. In this case the response matrix of one of the instruments may be adjusted by uniformly multiplying it with a constant. The other situation occurs for off-axis or extended sources, observed with collimated instruments. The multiplication factor may then be the collimator correction.

OPT Optimise the response and data for fitting purposes

This option deletes all channels with zero data errors and all input energy grid bins with zero response. During spectral fitting, zero data errors will result in an endless loop with infinite χ^2. However, it is better to rebin the spectrum first before optimizing it.

Table 3.1: Output of the SPEX show data option.

Latest spectral data file	...
Latest spectral response file	...
Number of photon model energy bins	#
Number of photon model energy bins	#
Number of response groups	#
Number of response groups	#
Photon model energy range (keV)	#
Data energy range (keV)	# ... #
Net source count rate (counts/s)	#
Net source counts	#
Background count rate subtracted(c/s)	#
Background counts subtracted	#
Average integration time per channel	#
Minimum integration time per channel	#
Maximum integration time per channel	#
Aver. exposure rat. source/background	#
Min. exposure ratio source/background	#
Max. exposure ratio source/background	#

Do **NOT** use this option if the current spectral model contains redshift components. In that case SPEX calculates it's model spectrum on a wider energy grid than that for which the detector may be sensitive.

BACK Back to previous menu

MAIN Back to main menu

SHOW Show the current data set

The ouput of this option is shown in tab. 3.1.

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3.4 Spectral model

The main menu options in this category enable the definition and modification of models that generate spectra that are to be compared with an observed spectrum. A model may consist of several additive and multiplicative components. The relations between the defined components can be changed at will. The various parameters of the spectral models can be modified as well.

MOD Modify the spectral model *mod*

In a spectral model SPEX uses two different types of components: *emission* and *absorption*, here called *additive* and *multiplicative* respectively. Additive components have a normalisation that determines

the flux level. Multiplicative components operate on additive components. A delta line or a power law are typical examples of additive components. Interstellar absorption is a typical example of multiplicative components. The redshift component is treated as a multiplicative one, since it operates on additive components.

ADD Define an additive component *moda*

See chapter 4 for specific information about the model components.

The newly defined component will be appended to the already existing one(s). A maximum number of 16 additive components is permitted.

- *POW* Simple power law
- *DELT* Delta line
- *CIE* Collisional ionisation equilibrium model
- *NEIJ* NEI model: discontinuous temperature jump
- *SED* SNR model: Sedov (adiabatic)
- *CHEV* SNR model: Chevalier (adiabatic, reverse shock)
- *HAM* SNR model: Hamilton (adiabatic, reverse shock, clumps)
- *SOLI* SNR model: Solinger et al. (isothermal)
- *BAND* SNR model: Band (isothermal or isentropic, reverse shock)
- *DEM* DEM model: differential emission measure analysis
- *MBB* Modified black body spectrum (MBB)
- *GAUS* Gaussian line
- *BB* Black body spectrum
- *BACK* Back to previous menu

MUL Define a multiplicative or redshift component *modb*

See chapter 4 for specific information about the model components.

The newly defined component will be appended to the already existing one(s). A maximum number of 8 multiplicative components is permitted.

- *REDS* Redshift component
- *ABSM* Absorption component (Morrison & McCammon)
- *EUVE* Absorption component (EUVE)
- *HOT* Absorption component (hot CIE medium)
- *BACK* Back to previous menu

Table 3.2: Output of the SPEX show model option.

```
Number of multiplicative components:
Nr.  01 :  multiplicative component name
                    ⋮
Nr.  ## :  multiplicative component name

Number of additive components:
Nr.  01 :  additive component name
                    ⋮
Nr.  ## :  additive component name
```

`DADD` Delete an additive component *modc*

After a component has been deleted, the remaining components will be renumbered.

- *##* Delete component ## (Ranging from 01 to 16)
- *BACK* Back to previous menu

`DMUL` Delete a multiplicative or redshift component *modd*

After a component has been deleted, the remaining components will be renumbered.

- *##* Delete component ## (Ranging from 01 to 08)
- *BACK* Back to previous menu

`REL` Set relation additive & multiplicative components *mode*

With this option it is possible to determine the way in which multiplicative components act on the additive components. For example, assume two multiplicative components: the first one an absorption and the second a redshift component. For each additive component the order in which the multiplicative components operate on it may be defined, e.g. first the redshift, then the absorption. In the above example the SPEX command would be `2,1,0,0,0,0,0,0`. It is also possible to enforce this relation on all defined additive components.

- *A##* Define relations for additive component ## (Ranging from 01 to 16)
- *SAME* Define the same dependence for all additive components
- *BACK* Back to previous menu

`SHOW` Show the current model

The output of this option is displayed in tab. 3.2.

`BACK` Back to main menu

PAR Modify the current model parameters *par*

The spectral model parameters of the current model may be adjusted with this main menu option. Select first the component, then the parameter and finally which property of the parameter should be modified in subsequent calls.

If one of the porperties of the same parameter as in the last call should be modified, the component and parameter need not to be defined again. Exception: in cases where the model has been adjusted by adding or deleting spectral model components.

COMP Select the spectral component *comp*

- *A##* Additive component ## (Ranging from 01 to 16)
- *M##* Multiplicative component ## (Ranging from 01 to 08)

PARA Select the parameter for the current component *para*

Depending on the current model and components:

- *POW* Simple power law *spow*
  - NORM Normalisation (10^{44} photons/s/keV at 1 keV)
  - GAMM Photon index
- *DELT* Delta line *sdel*
  - NORM Normalisation (10^{44} photons/s)
  - E Line energy (keV)
- *CIE* Collisional ionisation equilibrium model *scie*
  - NORM Normalisation = $n_e n_H$ V (10^{64}/m^3)
  - T Electron temperature (keV)
  - ED Electron density (10^{20}/m^3)
  - IT Ion temperature (keV)
  - VMIC Micro turbulence velocity (km/s)
  - ## Abundance of element ##, ranging from 02 to 30 (Z = 2 to 30)
- *NEIJ* NEI model: discontinuous temperature jump *snei*
  - NORM Normalisation = $n_e n_H V$ (10^{64}/m^3)
  - T1 Preshock electron temperature (keV)
  - T2 Postshock electron temperature (keV)
  - U Ionisation parameter (10^{20} s/m^3)
  - ED Electron density (10^{20}/m^3)

- IT — Ion temperature (keV)
- VMIC — Micro turbulence velocity (km/s)
- ## — Abundance of element ##, ranging from 02 to 30 (Z = 2 to 30)

SED SNR model: Sedov (adiabatic) *ssed*

- NORM — Normalisation (10^{20}/m^5)
- T — Electron temperature (keV)
- U — Ionisation parameter (10^{20} s/m^3)
- IT — Ion temperature (keV)
- VMIC — Micro turbulence velocity (km/s)
- S — Density gradient s of ISM
- NE — Density gradient n of stellar ejecta
- GAMM — Adiabatic index
- F — Angular filling factor
- PT — Pre-shock electron temperature (keV)
- NS — Number of shells
- NR — Number of projected rings
- EMIN — Minimum energy (keV) of radial profile
- EMAX — Maximum energy (keV) of radial profile
- RMIN — Minimum radius for projected spectrum annulus
- RMAX — Maximum radius for projected spectrum annulus
- ## — Abundance of element ##, ranging from 02 to 30 (Z = 2 to 30)

CHEV SNR model: Chevalier (adiabatic, reverse shock) *sche*

- NORM — Normalisation (10^{20}/m^5)
- T — Electron temperature (keV)
- U — Ionisation parameter (10^{20} s/m^3)
- IT — Ion temperature (keV)
- VMIC — Micro turbulence velocity (km/s)
- S — Density gradient s of ISM
- NE — Density gradient n of stellar ejecta
- GAMM — Adiabatic index
- F — Angular filling factor
- PT — Pre-shock electron temperature (keV)
- NS — Number of shells
- NR — Number of projected rings

- EMIN Minimum energy (keV) of radial profile
- EMAX Maximum energy (keV) of radial profile
- RMIN Minimum radius for projected spectrum annulus
- RMAX Maximum radius for projected spectrum annulus
- ## Abundance of element ##, ranging from 02 to 30 (Z = 2 to 30)

HAM SNR model: Hamilton (adiabatic, reverse shock, clumps) *sham*

- NORM Normalisation (10^{20}/m^5)
- T Electron temperature (keV)
- U Ionisation parameter (10^{20} s/m^3)
- IT Ion temperature (keV)
- VMIC Micro turbulence velocity (km/s)
- S Density gradient s of ISM
- NE Density gradient n of stellar ejecta
- ALFA Alpha parameter of Hamilton
- NU Nu parameter of Hamilton
- F Angular filling factor
- PT Pre-shock electron temperature (keV)
- NS Number of shells
- NR Number of projected rings
- EMIN Minimum energy (keV) of radial profile
- EMAX Maximum energy (keV) of radial profile
- RMIN Minimum radius for projected spectrum annulus
- RMAX Maximum radius for projected spectrum annulus
- ## Abundance of element ##, ranging from 02 to 30 (Z = 2 to 30)

SOLI SNR model: Solinger et al. (isothermal) *ssol*

- NORM Normalisation (10^{20}/m^5)
- T Electron temperature (keV)
- U Ionisation parameter (10^{20} s/m^3)
- IT Ion temperature (keV)
- VMIC Micro turbulence velocity (km/s)
- S Density gradient s of ISM
- NE Density gradient n of stellar ejecta
- GAMM Adiabatic index
- F Angular filling factor

- PT — Pre-shock electron temperature (keV)
- NS — Number of shells
- NR — Number of projected rings
- EMIN — Minimum energy (keV) of radial profile
- EMAX — Maximum energy (keV) of radial profile
- RMIN — Minimum radius for projected spectrum annulus
- RMAX — Maximum radius for projected spectrum annulus
- ## — Abundance of element ##, ranging from 02 to 30 (Z = 2 to 30)

BAND SNR model: Band (isothermal or isentropic, reverse shock) *sban*

- NORM — Normalisation (10^{20}/m^5)
- T — Electron temperature (keV)
- U — Ionisation parameter (10^{20} s/m^3)
- IT — Ion temperature (keV)
- VMIC — Micro turbulence velocity (km/s)
- S — Density gradient s of ISM
- NE — Density gradient n of stellar ejecta
- GAMM — Adiabatic index
- F — Angular filling factor
- PT — Pre-shock electron temperature (keV)
- NS — Number of shells
- NR — Number of projected rings
- EMIN — Minimum energy (keV) of radial profile
- EMAX — Maximum energy (keV) of radial profile
- RMIN — Minimum radius for projected spectrum annulus
- RMAX — Maximum radius for projected spectrum annulus
- ## — Abundance of element ##, ranging from 02 to 30 (Z = 2 to 30)

DEM DEM model: differential emission measure analysis *sdem*

- T1 — Lower electron temperature (keV)
- T2 — Upper electron temperature (keV)
- NR — Number of temperature bins
- IT — Ion temperature (keV)
- VMIC — Micro turbulence velocity (km/s)
- ED — Electron density (10^{20}/m^3)
- ## — Abundance of element ##, ranging from 02 to 30 (Z = 2 to 30)

MBB Modified black body spectrum (MBB) *smbb*

- NORM Normalisation (10^{26} m$^{0.5}$)
- T Temperature (keV)

GAUS Gaussian line *sgau*

- NORM Normalisation (10^{44} photons/s)
- E Line energy (keV)
- F Line width (FWHM, keV)

BB Black body spectrum (BB) *sbb*

- NORM Normalisation (10^{16} m$^{0.5}$)
- T Temperature (keV)

REDS Redshift component *sred*

- Z Redshift

ABSM Absorption component (Morrison & McCammon) *sabs*

- NH Hydrogen column density (10^{28}/m^2 = 10^{24}/cm^2)

EUVE Absorption component (EUVE) *seuv*

- NH Hydrogen column density (10^{28}/m^2 = 10^{24}/cm^2)
- HE1 He I / H I ratio
- HE2 He II / H I ratio

HOT Absorption component (hot CIE medium) *shot*

- NH Hydrogen column density (10^{28}/m^2 = 10^{24}/cm^2)
- T Electron temperature (keV)
- ## Abundance of element ##, ranging from 02 to 30 (Z = 2 to 30)

TYPE Select the type: value, status, step, min, max *paty*

With this option the properties of a spectral model parameter may be modified.

VAL Value of the parameter

The value of the parameter may be changed. Only values between the minimum and maximum values are accepted.

STAT Status of the parameter

The status of the parameter may be changed. 0 indicates a *frozen* parameter that will not change during a fitting procedure. 1 indicates a *free parameter* that may be changed during a fitting procedure.

STEP Step for the parameter

The stepsize used for determining the derivative of the model spectrum with respect to the parameter may be changed. This may be helpfull when convergence problems occur.

LOW Minimum for the parameter

UPP Maximum for the parameter

RSET Coupling of the parameter to another parameter

During spectral fitting, a parameter p_i may be coupled to another parameter p_j, maintaining always $p_i = c_{ij} p_j$ with c_{ij} the coupling constant, regardless of what p_j will be. A value of `0` indicates a parameter that does not depend upon other parameters. A positive value indicates the label j of the parameter to which p_i is coupled. This label is the unique number, indicated in the first column (with header par) that is displayed if the parameters are shown (option SHOW of this menu). The coupling constant is by default 1, unless another value is chosen using the XSET option of this menu.

XSET Coupling constant of the parameter to another parameter

This option allows to modify the coupling constant between coupled parameters (see above).

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VAL Set new values for the current parameter

SHOW Show the current parameters

The output of this option is shown in tab. 3.3.

RCOR Show the correlations between the fitted parameters

The output of this option is shown in tab. 3.4.

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3.5 Evaluation

CALC Evaluate the current spectral model

The currently defined spectral model is evaluated. If a spectral data set is present, the spectral model is convolved with the response matrix and the χ^2 is evaluated.

3.6 Simulation

SIM Simulate a spectrum using current model & detector *sim*

Table 3.3: Output of the SPEX option show current parameters. In this case the spectral model consists of two components. An additive collisional ionisation equilibrium model (cie) and a multiplicative absoprtion component (Morrison & McCammon) (absm).

```
-------------------------------------------------------------------------------
 mod  nr t parameter with unit     value     st      step    minimum   maximum

 cie   1 0 ne nH V (1E64/m**3)   9.92346E-06  1  1.00E-03 -1.00E+20  1.00E+20
 cie   2 2 Temperature (keV)      2.5186      1  1.00E-03  1.00E-04  1.00E+03
 cie   3 2 El. dens (1E20/m**3)  1.00000E-04  0  1.00E-03  1.00E-22  1.00E+10
 cie   4 3 Ion temp. (keV)        1.0000      0   .00E+00  1.00E-04  1.00E+07
 cie   5 2 Microturb vel (km/s)   .00000E+00  0   .00E+00   .00E+00  3.00E+05
 cie   6 1 Abundance He           1.0000      0  1.00E-03 -1.00E+10  1.00E+10
 ...            ...                ...       .     ...       ...       ...
 cie  34 1 Abundance Zn           1.0000      0  1.00E-03 -1.00E+10  1.00E+10
 absm  1 2 Column (1E28/m**2)    1.37425E-04  1  1.00E-03   .00E+00  1.00E+10
-------------------------------------------------------------------------------
 Fluxes and restframe luminosities between   .20000     and    12.000     keV

  nr mod   photon flux   energy flux nr of photons    luminosity
         (phot/m**2/s)      (W/m**2)   (photons/s)          (W)
   1 cie    82.235      1.49219E-14  1.02189E+39  1.63844E+23
 Chi-squared value :       888.76
 Degrees of freedom:   324
```

Notation: nr denotes the parameter number of the model component. t is a model specific parameter that defines the type of the parameter. t ranges from 0 to 3. 0 = normalization parameter; 1 = abundance paramter; 2 = fit parameter; 3 = non fit parameter. st denotes the status of the parameter. 0 = frozen; 1 = fittable. Each parameter may be fitted (if allowed) in the range between minimum and maximum with stepsize step.

Table 3.4: Output of the SPEX option show the correlation between the fitted parameters. In this case the spectral model consists of two components. An additive collisional ionisation equilibrium model (`cie`) and a multiplicative absoprtion component (Morrison & McCammon) (`absm`).

```
------------------------------------------------------------------------
 mod  nr parameter with unit   mod  nr parameter with unit   correlation

 cie   2 Temperature (keV)     cie   2 Temperature (keV)       1.0000
 cie   2 Temperature (keV)     absm  1 Column (1E28/m**2)     -.99999
 absm  1 Column (1E28/m**2)    absm  1 Column (1E28/m**2)      1.0000
------------------------------------------------------------------------
 mod  nr parameter with unit   mod  nr parameter with unit   correlation

 cie   1 ne nH V (1E64/m**3)   cie   1 ne nH V (1E64/m**3)     1.0000
```

With this main menu option SPEX will simulate a spectrum based on the currently defined spectral model and the chosen detector. SPEX will do the simulation based on the parameters as displayed in the menu below. These parameters have to be set **before** doing the actual simulation.

SPEX's simulation procedure is briefly as follows. First the total spectrum in the source region is calculated, including source and background counts. The total number of counts is randomized, using Poisson statistics. The background spectrum in the background region is evaluated and randomized. Then this background is scaled to the expected value in the source region and substracted from the 'raw' source spectrum.

SPEX always saves the expected background contribution in the source region (not randomized) to the spectral file (if the simulated spectrum is saved). This in order to enable further simulations using the currently simulated spectrum as a template.

It may occur that the spectrum used as a template for spectral simulation consists of data from more than one instrument. In that case SPEX can simulate a new spectrum provided that:

1. The integration times for all instruments are the same.
2. The systematic errors should be the same for all instruments.
3. The ratio of source-to-background area will **not** be changed!

In all other cases the instrument spectra should be simulated individually before being added together.

`SUB` Subtract background (yes or no)

SPEX always uses background substracted spectra. However if 'raw' spectra (background included) are to be simulated, SPEX offers a possibility to simulate them here. These spectra are not to be fitted with SPEX.

Default at program startup is: yes.

`AREA` Set ratio source-to-background area

If this ratio is very small, the background can be determined very accurately. However, note that for most instruments very large background areas may introduce systematic errors in the background estimate for the source region, due to variations in detector response to background counts. For imaging detectors this is the ratio of the number of pixels in the source and in the background region (if necessary corrected for small detector inhomogeneities). For collimator detectors this ratio should be 1, since the background is determined by swapping the detector between source and background.

The source-to-background area ratio may be energy-dependent e.g. for imaging detectors with energy-dependent spatial pointspread functions such as the SAX-ME concentrator. In this case SPEX reads the new ratio for the first channel ($R_{\mathrm{new},1}$) and calculates the new ratio for channel i by:

$$R_{\mathrm{new},i} = R_{\mathrm{old},i} \frac{R_{\mathrm{new},1}}{R_{\mathrm{old},1}}. \tag{3.1}$$

`TIME` Integration time source spectrum

Default at program startup is: 40000 s.

`BTIM` Integration time background spectrum

Default at program startup is: 40000 s.

`NOIS` Add Poisson noise (yes or no)

Realistic spectra require Poisson noise.

Default at program startup is: yes.

`SYST` Systematic error (fraction of source flux)

This option is useful in cases where the detector efficiency is variable in time or badly calibrated and when these variations cannot be reproduced. SPEX uses the systematic errors as being energy-independent.

Default at program startup is: 0.

`BSYS` Systematic error (fraction of raw background)

This option is useful in cases where the detector background is time variable or is different for the source and background region and can not be reproduced. SPEX uses the systematic errors as being energy-independent.

Default at program startup is: 0.

`RUN` Do the simulation

`MAIN` Back to main menu

3.7 Fitting

The main menu options in this category provide possibilities to fit the spectral model on the selected data.

FIT Fit the parameters using current data & model *fit*

With this main menu option the spectral model may be fitted to the selected data, using the spectral fitting method defined by menu option METH .

METH Change the spectral fitting method *ftyp*

CLAS Fit the spectrum (classical Levenberg-Marquardt method)

This widely used method is a combination of the steepest descent and the inverse Hessian method (See Press et al.). It is well known that this method does not always converge to the absolute minimum, but sometimes to a local sub-minimum. This method is used in the DEM analysis, since it does not use a normalization.

LML Fit the spectrum (Levenberg-Marquardt & linear scalings)

As above, however the normalizations and abundances of the additive components are determined by simple matrix inversion. All abundances are determined in a single iteration step which speeds up the calculations considerably.

☞ This method should **not** be used in combination with a DEM analysis, because it uses a normalization!

SIML Fit the spectrum (Simplex & linear scalings)

This method is based on the Simplex minimization method by Press et al. This method is not yet available in the current version of SPEX. It should be used for complicated cases.

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CHI Set weighting type for χ^2 calculation *ftyp*

DATA Use data errors in weights (classical chi**2 method)

This is the most widely used method. χ^2 is usually calculated as the sum over all data bins i of $(N_i - s_i)^2/\sigma_i^2$ where N_i is the observed number of source plus background counts, s_i the expected number of source plus background counts of the fitted model, and for Poisson statistics usually one takes $\sigma_i^2 = N_i$. Take care that the spectral bins contain sufficient counts (either source or background), recommended is e.g. to use at least ~10 counts per bin. If this is not the case, first rebin the data set.

☞ The method has inaccuracies if N_i is less than ~100. In that case, use *MOD* (see below).

MOD Use source + background model counts in weights

Wheaton et al. (1995) have shown that the classical χ^2 method becomes inaccurate for spectra with less than $\sim$ 100 counts per bin. This is *not* due to the approximation of the Poisson statistic by a normal distribution, but due to using the *observed* number of counts N_i as weights in the calculation of χ^2. Wheaton et al. showed that the problem can be resolved by using instead $\sigma_i^2 = s_i$, i.e. the *expected* number of counts from the best fit model. The current option allows to use these modified weights. By selecting it, the expected number of counts (both source plus background) of the current spectral model is used onwards in calculating the fit statistic. Wheaton et al. suggest to do the following 3-step process, which we also recommend to the user of SPEX: first fit the spectrum using the data errors as weights (option *DATA*, the default at start-up of SPEX). After completing this fit, select the *MOD* option and do again a fit; then repeat this step once more by again selecting *MOD* in order to replace s_i of the first step by s_i of the second step in the weights. The result should now have been converged (under the assumption that the fitted model gives a reasonable description of the data).

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RUN Fit the parameters using current data & model

ERR Determine error bounds on parameters *err*

It is possible to determine the error bounds on one spectral model parameter at a time. SPEX determines the error bounds by iteratively modifying the parameter of interest and calculating χ^2 as a function of the parameter. During this process the other free parameters of the model may vary. The iteration stops when $\chi^2 = \chi^2_{\rm min} + \Delta\chi^2$, where $\Delta\chi^2$ is a parameter that can be set separately. The iteration steps are displayed. It is advised to check them, because sometimes the fit at a trial parameter converges to a different solution branch, therefore creating a discontinuous jump in χ^2. In those situations it is better to find the error bounds by using the step option or by varying the search parameter by hand.

COMP Select the spectral component for error search *comp*

A## Additive component ## (Ranging from 01 to 16)

M## Multiplicative component ## (Ranging from 01 to 08)

PARA Select the parameter for the current component *para*

See §3.3 under **PARA**.

DCHI Set level of $\Delta\chi^2$ for the errors

The default value is 2. This is 1σ for one parameter of interest. For other values see tab. 3.5.

RUN Determine the errors

SPEX calculates the positive and negative error bounds separately.

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Table 3.5: $\Delta\chi^2$ as a function of confidence level and degrees of freedom. # is the number of parameters of interest for which the confidence level is calculated simultaneously, in general less than the number of free parameters. p is the probability of the confidence level. In case of doubt, take 1 parameter of interest.

	# parameters of interest					
p	1	2	3	4	5	6
1σ	2.00	4.00	6.00	8.00	10.00	12.00
68.3%	1.00	2.30	3.53	4.72	5.89	7.04
90%	2.71	4.61	6.25	7.78	9.24	10.6
95.4%	4.00	6.17	8.02	9.70	11.3	12.8
99%	6.63	9.21	11.3	13.3	15.1	16.8
99.73%	9.00	11.8	14.2	16.3	18.2	20.1
99.99%	15.1	18.4	21.1	23.5	25.7	27.8

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STEP Do a grid search *step*

A grid search is performed of χ^2 versus 1, 2, 3 or 4 parameters. The minimum, maximum and number of steps for each parameter may be adjusted. Steps may be linear or logarithmic. For each set of parameters, a spectral fit is made, using the last spectral fit before this STEP option as the starting point. For each step, the parameters and χ^2 are displayed. This option is useful in case of doubt about the position of the best fit in the parameter space, or in cases where the usual error search is complicated.

DIM Dimension of grid (number of search parameters)

Default at program startup is: 1.

Set parameters for # parameter axis in grid search (Ranging from 1 to 4)

COMP Select the spectral component for current axis *ste1* ... *ste4*

A## Additive component ## (Ranging from 01 to 16)

M## Multiplicative component ## (Ranging from 01 to 08)

PARA Select the parameter for the current component and axis

See §3.3 under PARA .

LOW Set lower value for parameters axis

UPP Set upper value for parameters axis

N Set number of steps for parameters axis (negative for log steps)

For example:

grid axis								axis type	input
1	2	3	4	5	6	7	8	lineair	8
1	2	4	8	16	32	64	128	logarithmic	-8

BACK Back to previous menu

MAIN Back to main menu

RUN Do the grid search

SPEX does the grid search and displays for each search parameter the following information:

```
Parameter value , Chi**2 , Delta chi**2 with respect to minimum
```

BACK Back to previous menu

MAIN Back to main menu

MAIN Back to main menu

DEM Differential Emission Measure analysis (DEM) *dem*

This main menu option provides tools to make a good DEM–analysis. DEM analysis should be used when the spectrum or model contains a continuous temperature distribution. The spectral model can only have one additive component: the DEM component that corresponds to a multi-temperature structure. There are no restrictions to the number of multiplicative components. For a description of the DEM analysis method see document SRON/SPEX/TRPB05 and Mewe et al. (1994).

Currently there are 2 DEM analysis methods available: the regularisation method (for which the options REG , DEM , SCAL , AUTO , CHIR are available), and the cleaning method, for which the option CLEA can be used. The options IN and SAVE can be used with both methods.

The options in this menu determine the emission measure distribution but perform no fitting of other spectral parameters. When the fitting of the other parameter is desired, the fit option of the main menu should be used. Note that in this case the fitting method should be the **classical** Levenberg & Marquardt method (without linear scalings). The DEM algorithm uses a second order regularisation, see document SRON/SPEX/TRPB05 and Mewe et al. (1994).

For both methods, *first* the library of convolved spectra should be generated using the LIB option.

It is important to use the right regularisation parameter!

LIB Generate the spectrum library

Calculate the library of convolved basis spectra for the DEM analysis.

LIB has to be executed again if any spectral parameter is changed, but not if only the regularisation is changed.

REG Set regularisation parameter

This option sets the regularisation parameter manually. Larger values correspond to more smoothing, 0 means no smoothing (but then the solution is unphysical). After this step, the DEM analysis can be performed by choosing DEM .

`DEM` Do the differential emission measure analysis using the regularisation method

With this option the differential emission measure (DEM) analysis may be performed on the current data set for the given regularisation parameter. The library of convolved spectra has been calculated before with `LIB` .

`SCAL` Set scale for automatic regularisation parameter search

With this option the scaling value f is set. It is used for the automatic regularisation. Default and recommended value is 1. In this case the regularisation R is determined by

$$\chi^2(R) = \chi^2(R=0)\left(1 + f\sqrt{\frac{2}{n_{\rm channel} - n_{\rm T}}}\right), \tag{3.2}$$

where f is the scaling factor, $n_{\rm channel}$ is the number of channels in the data set and $n_{\rm T}$ is the number of temperature components.

`AUTO` Automatic search for optimum regularisation & DEM analysis

This option automatically chooses the optimal regularisation parameter using eq. (3.2) and performs the DEM analysis. Usually this procedure is satisfactory. Sometimes the result is not satisfactory and manual regularisation should be used, followed by `DEM` .

`CHIR` Make a list of χ^2 versus regularisation parameter *chir*

LOW Set lower value for regularisation

UPP Set upper value for regularisation

N Set number of steps for regularisation (neg. for log steps)

For example:

grid								grid type	input
1	2	3	4	5	6	7	8	lineair	8
1	2	4	8	16	32	64	128	logarithmic	-8

RUN Make a list of χ^2 versus regularisation parameter

For each selected regularisation parameter, SPEX lists the χ^2 value, and the DEM–penalty p, which is defined by

$$p = \sum_{y_i<0}\left(\frac{y_i}{\Delta y_i}\right)^2, \tag{3.3}$$

where y_i is the emission measure of temperature bin i and Δy_i it's error. For a physical acceptable solution p should not be much larger than half the number of temperature bins.

BACK Back to previous menu

MAIN Back to main menu

`IN` Read a model DEM distribution and evaluate that model

SPEX asks for a filename without the extension `.dem`.

`SAVE` Save the DEM distribution to an ascii file

SPEX asks for a filename without the extension `.dem`.

`CLEA` Do the differential emission measure analysis (clean method)

`MAIN` Back to main menu

3.8 Plots & ASCII files

This category handles the presentation of the calculated data. Plots may be made in the form of graphical output or alternatively written as PostScript files. Data may be written to ASCII files.

ASC Output of SPEX model properties to file or screen

With this main menu option SPEX's current model properties can be displayed either on screen or saved into an ASCII file.

Only components corresponding with plasma models can be used in this main menu option.

Before displaying the menu structure, SPEX will recalculate the current model. This is because during normal model evaluations not all the necessary model information is calculated, because of numerical efficiency reasons.

`COMP` Select the spectral component *comp*

- *A##* Additive component ## (Ranging from 01 to 16)
- *M##* Multiplicative component ## (Ranging from 01 to 08)

`DEV` Output to screen or file

`NAME` Give file name for ascii output (without .asc)

`TYPE` Select the type of output *asub*

- *CPU* Run time statistics
- *PLAS* Plasma parameters (temperatures, densities etc.)
- *HEAT* Heating and cooling rates
- *ABUN* Abundances & average charge ions
- *ICON* Ion concentrations
- *RION* Ionisation rates per ionic subshell

- *RATE* Ionisation and recombination rates per ion
- *GRID* Energy grid used for calculation of the model
- *CON* Continuum emission components (ff, fb, 2p & total) for layer
- *CLIN* Continuum and total line radiation spectrum for layer
- *LINE* Spectral line fluxes for layer
- *EBAL* Energy balance loop control parameters
- *SNR* Supernova Remnant parameters
- *TCON* Total continuum emission components (ff, fb, 2p & total)
- *TCL* Total continuum and total line radiation spectrum
- *TLIN* Total spectral line fluxes
- *CNTS* Calculate expected line counts for current model & detector
- *BACK* Back to previous menu
- *MAIN* Back to main menu

RUN Give the requested output

MAIN Back to main menu

PLOT Plot menu *pmen*

This main menu option provides the possibility to make plots of data and models processed by SPEX. The pgplot interface is used for this purpose. The plot menu options cover nearly all the desirable features one may find in various other packages e.g. IDL. However, if special plot features are required, one is advised to save the respective data sets and use a different plot package.

A plot type should be selected before the actual plot is made. Once a plot type is selected, it will be used until another type is selected.

TYPE Select a new plot type *ptyp*

Each plot type distinguishes a **data** and a **model** part. The model part may consist of different components. The data and model parts are indicated for the plot types listed below.

The options *COMP*, *SPEC* and *TY* may only be selected when the current spectrum model contains plasma components.

COMP Select a plasma component for plotting *comp*

- *A##* Additive component ## (Ranging from 01 to 16)
- *M##* Multiplicative component ## (Ranging from 01 to 08)

Table 3.6: Line styles for the continuum and line emission components (initially).

free-free emission	- - - - -
free-bound emission	.-.-.-.-.-
two photon	. . . . .
total continuum	----------
line emission	(not plotted)

DATA Observed spectrum & predicted model

The observed spectrum convolved with the instrument response is plotted as data and the convolved model spectrum as model.

MOD Model photon spectrum

The photon spectrum is plotted as data.

AREA Effective area of the detector

Effective area of the detector is plotted as data.

RESP Response matrix

The response matrix is plotted as a two dimensional map. The abscis displays the channel number, the ordinate displays the input energy bin number.

CHI2 Fit residuals

The fit residuals are plotted as data. The line $y = 0$ is plotted as model.

SPEC Plasma model: Continuum and line emission components

The total component spectrum is plotted as data and the model is plotted with the linestyles displayed in tab. 3.6.

TY Plasma model: Emission measure versus temperature

The emission measure is plotted as data. Only when an input DEM was read, this input DEM is plotted as model.

MAIN Back to main menu

PLOT Do the plot

SPEX plots the plot with all current settings on the selected output device. An example plot is given in fig. 3.4.

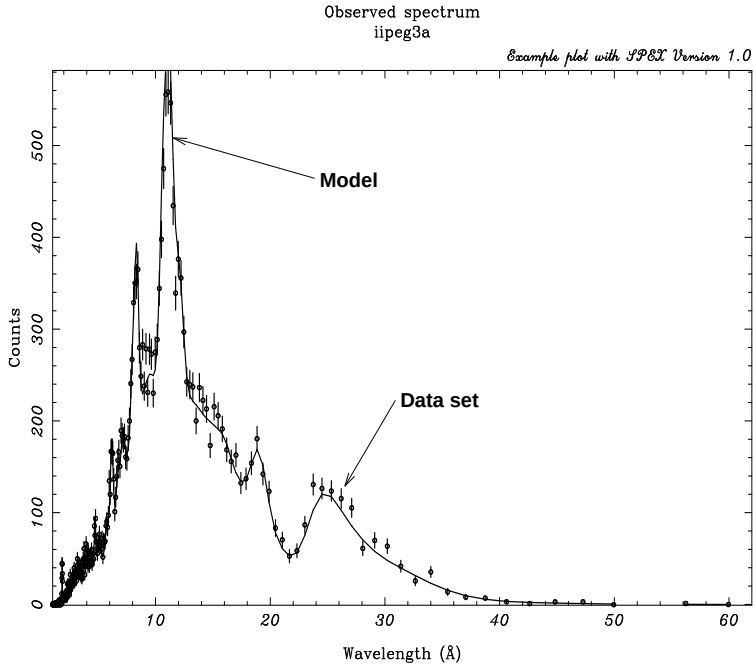
The available output devices depend on the available output devices in the pgplot library that is used by SPEX.

DEV Set plotting device *pdev*

NULL Null device, no output

PS PostScript file, landscape orientation

Default at program startup is: spex.



Plot characteristics

plot type	: data (observed spectrum & predicted model)
plot device	: PostScript file (landscape orientation)
x–axis units y–axis units	: Wavelength (Å) : Counts
font for box annotation font for x & y–axis label font for upper & lower title label font for identification label	: italic : roman : roman : script
x–axis label y–axis label upper title label lower title label identification label	: `Wavelength (Å)`, (generated by SPEX) : `Counts`, (generated by SPEX) : `Observed spectrum`, (generated by SPEX) : `iipeg3a`, the name of the data set (generated by SPEX) : `Example plot with SPEX Version 1.0`, (modified)
plot symbol (data)	: single error bar with plot symbol 21 (○)
line plot mode	: continuous line plot mode for model
line weight for x & y–axis label line weight for upper title lable line weight for data & model	: 2 (i.e. bold face) : 2 (i.e. bold face) : 3

Figure 3.4: Example plot with SPEX Version 1.0, PostScript (landscape orientation). The plot characteristics that were changed from the default values at program startup, are also shown.

VPS PostScript file, portrait orientation

Default at program startup is: spex.

CPS Colour PostScript file, landscape orientation

Default at program startup is: spex.

VCPS Colour PostScript file, portrait orientation

Default at program startup is: spex.

TEK Tektronix 4010 terminal

GF GraphOn Tek terminal emulator

RETR Retrographics VT640 Tek emulator

XTER XTERM Tek terminal emulator

XWIN Window on Xwindow server

XDIS Pgdisp or figdisp server

X11 X11

NAME Set plot file name

 This option need only to be selected in case a hardcopy device is used (e.g. PostScript). SPEX will ask for a file name.

HLAN PostScript print (landscape mode)

HPOR PostScript print (portrait mode)

LX Change x-axis scale scale logarithmic / linear

LY Change y-axis scale scale logarithmic / linear

LZ Change z-axis scale scale logarithmic / linear

UX Redefine x-axis units

When **TYPE** is *DATA, MOD, AREA, CHI2, SPEC*: *uxda*

BIN Bin nr.

KEV Energy (keV)

RYD Energy (Rydberg)

HZ Frequency (Hz)

ANG Wavelength (Å)

NM Wavelength (nm)

M Wavelength (m)

When TYPE is *RESP*: *uxrp*

BIN Channel nr.

When spectral model type is *DEM*: *uxty*

BIN Bin nr.
KEV Temperature (keV)
DK Temperature (K)
MK Temperature (MK)

UY Redefine y-axis units

When TYPE is *DATA*: *uyda*

BIN Bin nr.
COU Counts
CS Counts/s
KEV Counts/s/keV
RYD Counts/s/Ryd
HZ Counts/s/Hz
ANG Counts/s/Å
NM Counts/s/nm
M Counts/s/m
FCS Counts/m^2/s
FKEV Counts/m^2/s/keV
FRYD Counts/m^2/s/Ryd
FHZ Counts/m^2/s/Hz
FANG Counts/m^2/s/Å
FNM Counts/m^2/s/nm
FM Counts/m^2/s/m

When TYPE is *MOD*: *uymo*

BIN Bin nr.

COU Photons/m^2/s/bin

KEV Photons/m^2/s/keV

RYD Photons/m^2/s/Ryd

HZ Photons/m^2/s/Hz

ANG Photons/m^2/s/Å

NM Photons/m^2/s/nm

M Photons/m^2/s/m

FWK Flux (W/m^2/keV)

FWHZ Flux (W/m^2/Hz)

FWA Flux (W/m^2/Å)

FWNM Flux (W/m^2/nm)

FJ Flux (Jy)

IW νF_ν (W/m^2)

IJ νF_ν (JyHz)

When TYPE is *AREA*: *uyar*

BIN Bin nr.

M2 Area (m^2)

CM2 Area (cm^2)

When TYPE is *RESP*: *uyrp*

BIN Energy bin nr.

When TYPE is *CHI2*: *uych*

DCHI $\Delta\chi$ = (obs - mod) / err

CS Counts/s

KEV Counts/s/keV

RYD Counts/s/Ryd

HZ Counts/s/Hz

ANG Counts/s/Å

NM Counts/s/nm

M Counts/s/m

When TYPE is *SPEC*: *uysp*

BIN Bin nr.

COU Emission (10^{44} Photons/s/bin)

KEV Emission (10^{44} Photons/s/keV)

RYD Emission (10^{44} Photons/s/Ryd)

HZ Emission (10^{44} Photons/s/Hz)

ANG Emission (10^{44} Photons/s/Å)

NM Emission (10^{44} Photons/s/nm)

M Emission (10^{44} Photons/s/m

FWK Power (10^{28} W/keV)

FWHZ Power (10^{28} W/Hz)

FWA Power (10^{28} W/Å)

FWNM Power (10^{28} W/nm)

IW Power νF_ν (10^{28} W)

When spectral model type is *DEM*: *uyty*

BIN Bin nr.

SPEX Y (10^{64}/m^3)

DSPE Y/d^2 (10^{20}/m5)

CMPC Y/d^2 (10^{50}/cm^3/p^2)

PSK dY/dT (10^{64}/m^3/keV)

PSD dY/dT (10^{64}/m^3/K)

PDK $(dY/dT)/d^2$ (10^{20}/m^5/keV)

PDD $(dY/dT)/d^2$ (10^{20}/m^5/K)

PCK $(dY/dT)/d^2$ (10^{50}/cm^3/pc^2/keV)

PCD $(dY/dT)/d^2$ (10^{50}/cm^3/pc^2/K)

UZ Redefine z-axis units

When TYPE is *resp*: *uzrp*

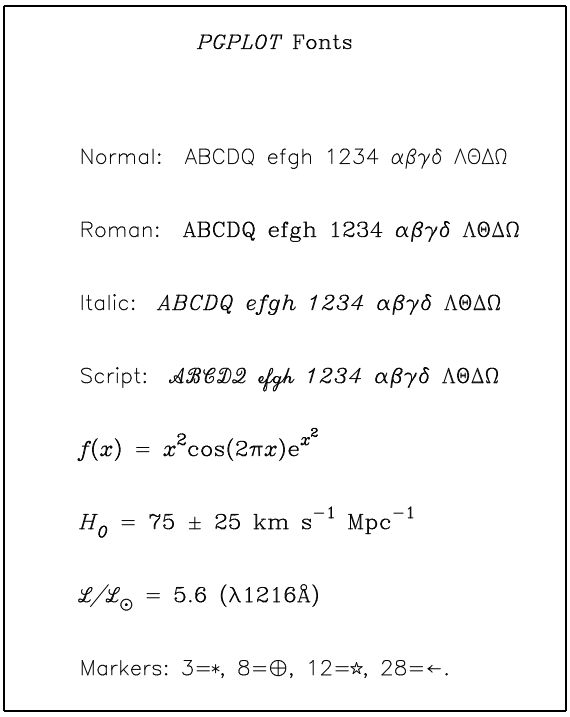


Figure 3.5: Example of available font types.

M2 Area / channel range (m^2/keV)

CM2 Area / channel range (cm^2/keV)

RX Modify x-axis range

RY Modify y-axis range

RZ Modify z-axis range

FONT Change font type

ALL Modify the font type for all character strings *pfon*

The available font types are shown in fig. 3.5.

NORM Normal

ROM Roman

ITA Italic

SCR Script

BOX Modify the font type for the box annotation only *pfon*

See options at *ALL* .

X Modify the font type for the x-axis label only *pfon*

See options at *ALL* .

Y Modify the font type for the y-axis label only *pfon*

See options at *ALL* .

UTIT Modify the font type for the upper title label only *pfon*

See options at *ALL* .

LTIT Modify the font type for the lower title label only *pfon*

See options at *ALL* .

ID Modify the font type for the identification label only *pfon*

See options at *ALL* .

FH Change font height *pfh*

Default at program startup is: 1, for all character strings. The font height may be chosen within the range from 0 (invisible) to 1000 (extremely large).

ALL Modify the font size for all character strings

BOX Modify the font size for the box annotation only

X Modify the font size for the x-axis label only

Y Modify the font size for the y-axis label only

UTIT Modify the font size for the upper title label only

LTIT Modify the font size for the lower title label only

ID Modify the font size for the identification label only

DATA Modify the font size for the data symbols only

CAP Modify caption texts *pcap*

The caption texts may be modified using the pgplot escape sequences. These are character–sequences that are not plotted, but are interpreted as instructions to change the font, draw superscripts or subscripts, draw non-ASCII characters, Greek letters, etc. All escape sequences start with a backslash character (\). A list of the defined escape sequences is given in tab. 3.7. A lookup table for Greek letters is presented in tab. 3.8. Some useful non-ASCII characters are listed in tab. 3.9. Fig. 3.6 shows some examples of the use of pgplot escape sequences in character strings.

X Modify the x-axis label

Y Modify the y-axis label

Table 3.7: A list of available escape sequences.

Seq.	description
`\u`	start a superscript or end a subscript. A `\u` must be ended by a `\d`!
`\d`	start a subscript or end a superscript. A `\d` must be ended by a `\u`!
`\\`	backspace (i.e. do not advance textpointer after plotting the previous character)
`\A`	Ångstrom symbol (Å)
`\g`x	greek letter corresponding to roman letter x
`\fn`	switch to Normal font
`\fr`	switch to Roman font
`\fi`	switch to Italic font
`\fs`	switch to Script font
`\(`n`)`	character number n, see *pgplot manual appendix B, tab. 1*

Table 3.8: List of upper- and lower case Greek letters (G) and their corresponding Roman letters (R).

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

Table 3.9: Some useful non-ASCII character sequences.

$\sim$	2248	$\pm$	2233	∇	0583
$\approx$	0248	$\mp$	2234	$\surd$	2267
$\cong$	0250	$\times$	2235	$\int$	2268
$\propto$	2245	$\div$	2237	$\oint$	2269
$\neq$	2239	$\equiv$	2240	∞	2270
$\leq$	2243	$\dagger$	2277	∂	2286
$\geq$	2244	$\ddagger$	2278	$\odot$	2281

Displayed	pgplot escape sequence
$f(x) = x^2 \cos(2\pi x)$	`\fif(x) = x\u2\d \frcos\fi(\fr2\fi\gpx)`
$H_0 = 75 \pm 25$ km s^{-1} Mpc^{-1}	`\fiH\d0\u\fr = 75 \(2233) 25 km s\u-1\d Mpc\u-1\d`
$\mathcal{L}/\mathcal{L}_\odot = 5.6$ (λ1216Å)	`\fsL/L\fr\d\(2281)\u = 5.6 (\gl1216\A)`

Figure 3.6: Some examples of the use of pgplot escape sequences.

UTIT Modify the upper title label

LTIT Modify the lower title label

ID Modify the identification label

SYMB Change plot symbols *psym*

NOT So not plot any symbol

BAR Single error bar

CROS Two crossed error bars

BS Single error bar with plot symbol

Default at program startup is: 17. Plot symbols may be chosen within the range from -8 to 31, see fig. 3.7.

CS Two crossed error bars with plot symbol

SYMB Plot symbol only

Default at program startup is: 17. Plot symbols may be chosen within the range from -8 to 31, see fig. 3.7.

HIS Histogram / continuous line plot mode *phis*

This menu option provides the possibilty to *switch* between histogram or continuous line plot mode.

DATA modify the plot mode for the data

MOD modify the plot mode for all model components

SING modify the plot mode for a single model component *pcom*

These are the components of the plot model, **not** the spectral model components!

Select component ## (Ranging from 01 to 32)

PGPLOT Marker Symbols

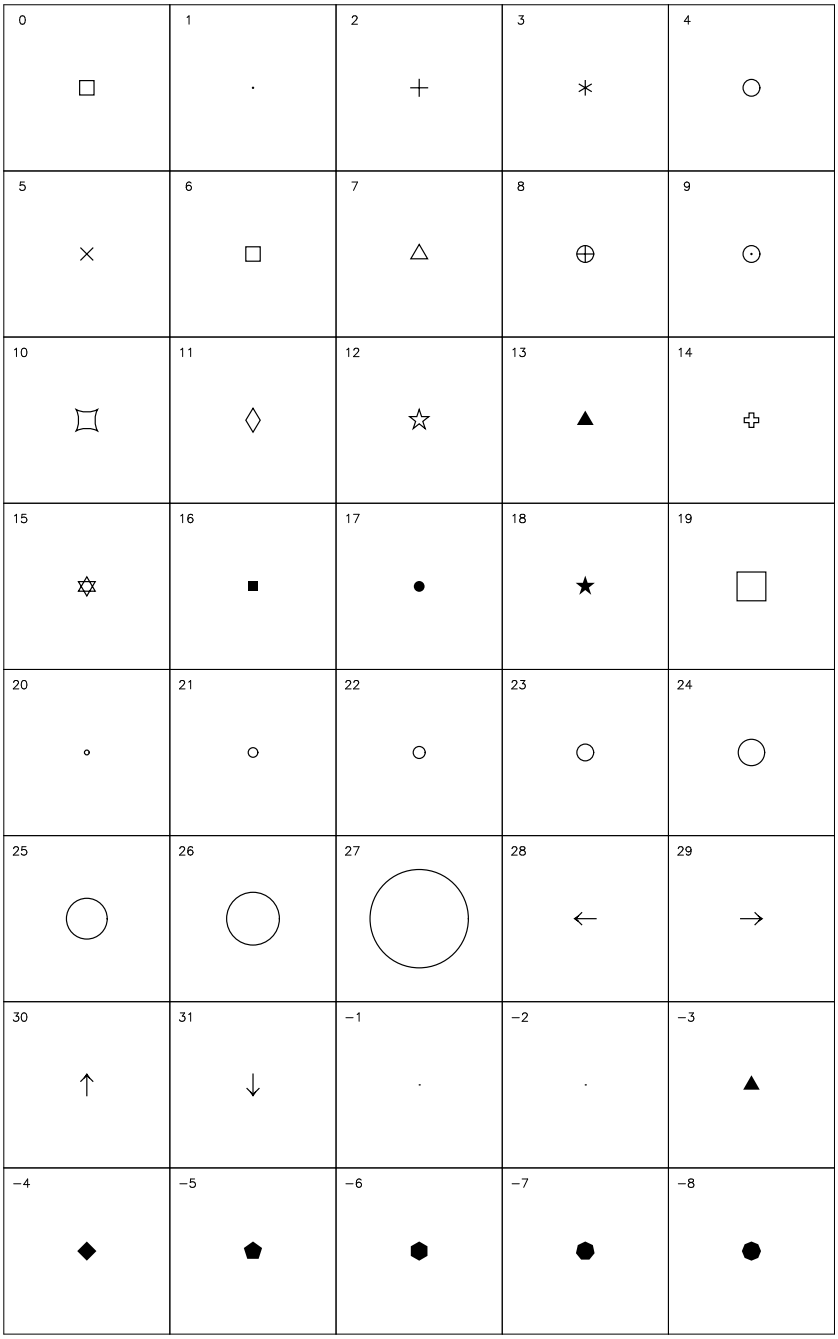


Figure 3.7: Example of available plot symbols.

LW Change line weights *plw*

Default at program startup is: 1. The line weights may be chosen within the range from 1 (normal) to 201 (extremely thick lines), see fig. 3.8.

Modifying the line weights of the labels may be used to generate **bold face** characters.

- *ALL* Modify the line weight for all plot variables
- *BOX* Modify the line weight for the box only
- *X* Modify the line weight for the x-axis label only
- *Y* Modify the line weight for the y-axis label only
- *UTIT* Modify the line weight for the upper title label only
- *LTIT* Modify the line weight for the lower title label only
- *ID* Modify the line weight for the identification label only
- *DATA* Modify the line weight for the data only
- *MOD* Modify the line weight for the model components only
- *SING* Modify the line weight for a single model component only *pcom*

  These are the components of the plot model, **not** the spectral model components!

  - ## Select component ## (Ranging from 01 to 32)

LT Change line styles *plt*

- *DATA* Modify the line style for the data *plts*
  - SKIP (do not plot)
  - CONT ----------
  - DASH - - - - - - -
  - PD .-.-.-.-.-.-.
  - DOT . . . . . .
  - DPP -..-..-..-..-
- *MOD* Modify the line style for all model components *plts*

  See options at *DATA* .
- *SING* Modify the line style for a single model component *pcom*

  These are the components of the plot model, **not** the spectral model components!

  - ## Select component ## (Ranging from 01 to 32)

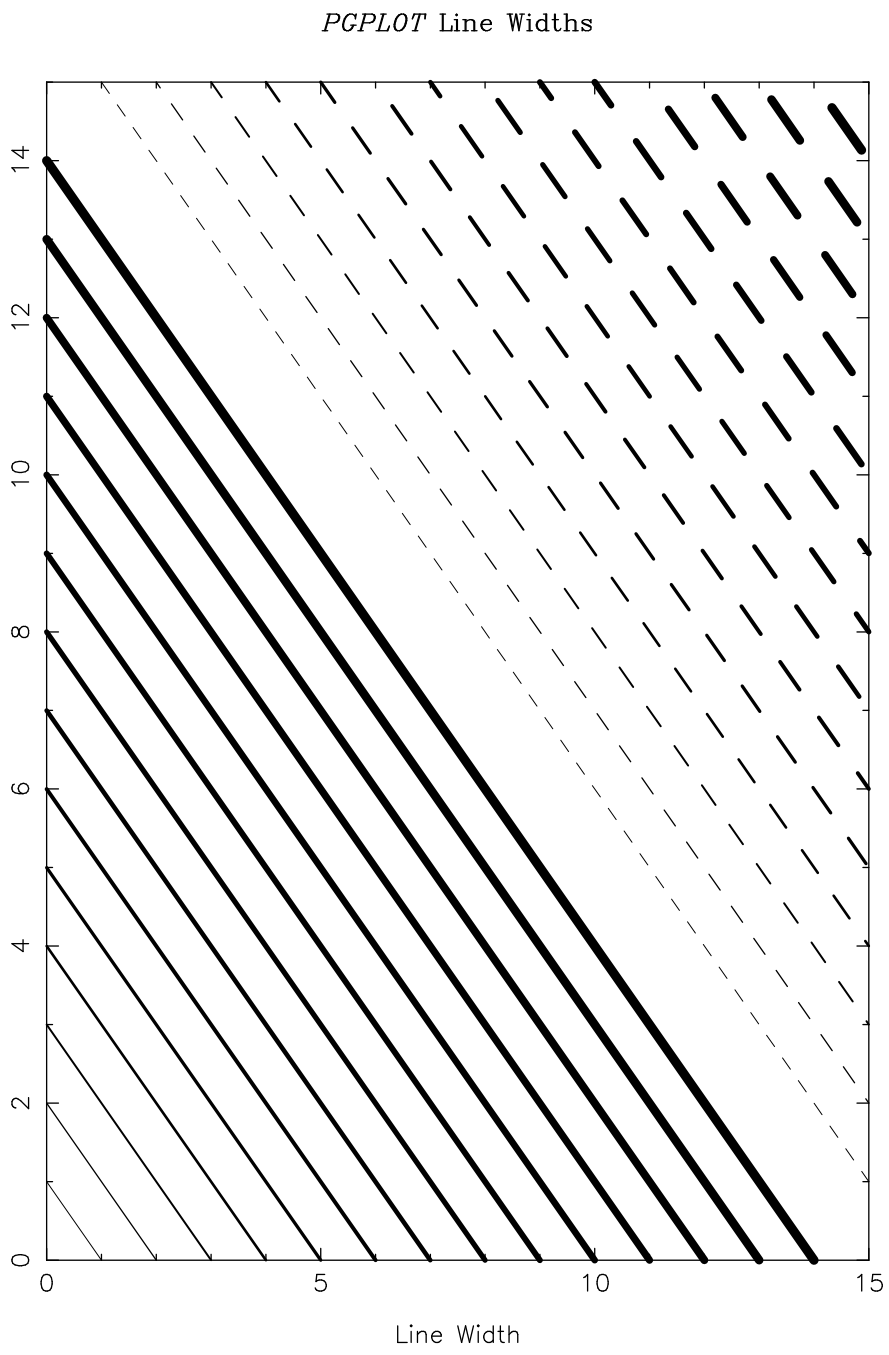


Figure 3.8: Example of available line weights.

Table 3.10: Available plot colours.

Value	Colour
01	Black (background)
02	White (default)
03	Red
04	Green
05	Blue
06	Cyan (Green + Blue)
07	Magenta (Red + Blue)
08	Yellow (Red + Green)
09	Orange (Red + Yellow)
00	Green + Yellow
11	Green + Cyan
12	Blue + Cyan
13	Blue + Magenta
14	Red + Magenta
15	Dark Gray
16	Light Gray

COL Change plot colours *pco*

ALL Modify the line colour for all plot variables *pcol*

Colour (Ranging from 01 to 16, see Tab. 3.10).

BOX Modify the line colour for the box only *pcol*

See Tab. 3.10.

X Modify the line colour for the x-axis label only *pcol*

See Tab. 3.10.

Y Modify the line colour for the y-axis label only *pcol*

See Tab. 3.10.

UTIT Modify the line colour for the upper title label only *pcol*

See Tab. 3.10.

LTIT Modify the line colour for the lower title label only *pcol*

See Tab. 3.10.

ID Modify the line colour for the identification label only *pcol*

See Tab. 3.10.

DATA Modify the line colour for the data only *pcol*

See Tab. 3.10.

MOD Modify the line colour for all model components *pcol*

See Tab. 3.10.

SING Modify the line colour for a single model component *pcol*

See Tab. 3.10.

GC Switch between gray-scale or contour plot


This option is only available in 2D plot mode e.g. *RESP*.

NC Change number of contour levels


This option is only available in 2D plot mode e.g. *RESP*.

CLEV Change contour levels

SPEX asks for the component number and it's new value.


This option is only available in 2D plot mode e.g. *RESP*.

MAIN Back to main menu

Chapter 4

SPEX Models

4.1 Introduction

The SPEX software encompasses a number of subroutines for the computation of emergent spectra based on a variety of plasma models such as optically thin plasmas in collisional ionization equilibrium (CIE), e.g. stellar coronal loop structures. Another category of optically thin plasmas are supernova remnants which show extreme transient ionization effects for which the non-equilibrium ionization (NEI) plasma model must be applied. Further we have photo-ionized plasmas, and optically thick plasmas. Single-, multi- and continous- temperature models are also available.

A synthetic spectrum program convolves the calculated input spectra with representative instrumental response functions which are described in the documents SRON/SPEX/TRIS01–05 for various instruments onboard current or future X-ray satellites.

Various applications can be classified for possible source configurations, for optically thin/thick plasmas, for single-, multi-, or continuous- temperature distributions and for steady-state or transient behaviour.

For a general description of various models we refer to the document SPEX/SRON/TRPB01 (shortly referred to as **PB01**), especially sections 3, 6, and 7, and for more specific descriptions to the cited literature. We distinguish between the following physical models:

1. **Power Law $E^{-\alpha}$ (nonthermal) spectrum** (α is the energy spectral index): For example, radiation from the core of Active Galactic Nuclei (AGN), or radiation from a solar flare.
2. **Delta function**, representing an infinitely narrow spectral line.
3. **Gaussian line**, representing a single spectral line broadened by e.g. thermal Doppler effects, by instrumental effects, or by turbulent velocities. We can make combinations of several lines.
4. **CIE model**: Optically thin, steady-state plasma in Collisional Ionization Equilibrium. The ionization and excitation occur by electron impact. The ionization is balanced by radiative and dielectronic recombination of an electron with an ion. The electron impact excitation of an ion or atom is generally followed by a spontaneous radiative transition between either two bound states, between two continuum states, or between a continuum and a bound state. The first process produces line radiation, the latter two ones produce free-free and free-bound continuum radiation. See also SRON/SPEX/TRPB01 and references therein. For line excitation processes, see SRON/SPEX/TRPB04 and appendices 04a–c ; for continuum radiation, see SRON/SPEX/TRPB03 ; for the ionization balance and processes, see SRON/SPEX/TRPB02.
5. **NEI model**: Discontinuous temperature jump causing Non-Equilibrium Ionization (transient optically thin plasmas such as solar flares and supernova remnants). The heating process (e.g. by a shock) yields a temperature rise so fast that the ionization cannot follow this. As a result, the ionization balance in the X-ray emitting plasma is generally far out of equilibrium. The same holds for cooling vs. recombination. See documents SRON/SPEX/TRPB01&02.

6. **DEM model**: Multi-temperature, optically thin plasma such as a stellar corona in steady-state or a supernova remnant (SNR) in transient state. The Diffferential Emission Measure (DEM) modelling uses theoretical reference spectra calculated in CIE. The DEM result generally does not reflect the true temperature distribution in the case of a SNR, but gives only an indication of the temperature regime. In the past we have applied several DEM modelling techniques, e.g., in solar flare analysis, in the analysis of *EXOSAT* transmission grating spectra of the coronae of several cool stars (e.g. Lemen et al. 1989), and very recently to the analysis of the *EUVE* spectra of a number of late-type stars (Mewe et al. 1994). In the document SRON/SPEX/TRPB05 we have described the modelling methods as applied in SPEX.

7. **SNR model**: SuperNova Remnant (optically thin, multi-temperature structure, transient state). The situation is prototype for a strongly NEI plasma. See PB01 and more specific for the various plasma models Kaastra and Jansen (1993). We distinguish between the following SNR models:

   - Sedov (adiabatic) model (Sedov 1959)
   - Chevalier (adiabatic, reverse shock) model (Chevalier 1982)
   - Hamilton (adiabatic, reverse shock, clumps) model (Hamilton 1985)
   - Solinger et al. (isothermal) model (Solinger et al. 1975)
   - Band (isothermal or isentropic, reverse shock) model (Band 1988)

   The Sedov and Solinger models describe only the outward blast shock wave ploughing through the interstellar matter, whereas the other models also take into account the inner reverse shock through the clumpy material from the remnant itself.

8. **(M)BB**: (Modified) Black-Body spectrum (e.g. from the region around an AGN; optically thick, single temperature). The BB spectrum is described by the Planck function, whereas the MBB spectrum is modified by inverse Compton scattering by nonrelativistic electrons in a dense medium (e.g., Rybicki and Lightman 1979) (see also PB01).

9. **Active-Region-Loop model**: Optically thin, multi-temperature, stationary plasma in coronal loop structures. In the past we have used the results from Vesecky et al. (1979) and Rosner et al. (1978) (see PB01), but in the future we will make use of the recent calculations by G.H.J. van den Oord. At the moment the model in SPEX is still TBD (and will be described in document SRON/SPEX/TRPB06).

10. **Hot high-gravity LTE atmosphere model**: Optically thick atmosphere with temperature stratification, in Local Thermal Equilibrium, with irradiation by an external radiation field (white dwarfs, accretion disks). This model has been developed by J. Heise (see also PB01 sec. 6.5.1, Heise et al.) during the past years and will be implemented later. At the moment the model in SPEX is still TBD (and will be described in document SRON/SPEX/TRPB07).

11. **Photo-ionized model**: Nebular type plasma with ionization dominated by an external radiation field (accretion disks in X-ray binaries). The ionization balance is set up between photo-ionization (instead of electron impact ionization) and radiative recombination. The model is currently under development by J.S. Kaastra (for some preliminary results, see PB01, section 6.4). At the moment the model in SPEX is still TBD (and will be described in document SRON/SPEX/TRPB08).

4.2 Spectral model parameters

In the future a list of all parameters (and default values at program startup) for each spectral model will be made available. At the moment we refer to the Cookbook (document SRON/SPEX/TRCB01) for a description of some spectral models and their relevant parameters.

4.3 Cookbook examples

In the Cookbook (document SRON/SPEX/TRCB01) we give a number of examples of spectral simulations using a so-called "log" file. We consider two categories of plasmas.

First, we deal with optically thin plasmas. In this category we consider the CIE equilibrium model applied to single-temperature fitting of various coronal plasmas (II Peg, Capella). We give an example of the DEM-modelling of a stellar coronal plasma which combines the physical properties of the hot star Capella and the relatively cooler, solar-type star α Centauri. We also calculate the NEI non-equilibrium model for a SNR and a more specific SNR (Chevalier) model for Cas A.

Secondly, for non-optically thin plasmas, we simulate for the case of an Active Galactic Nucleus (AGN) a model spectrum which combines a variety of features that is contained within SPEX: a red-shifted source with a spectrum that combines a power law, a modified blackbody, a CIE plasma, and a Gaussian spectral emission line. Moreover, in addition to the foreground absorption, a warm absorber is introduced.

It is our purpose to continuously extend and update the cookbook and we encourage every user to supply us with more examples!

Chapter 5

Instrumental Response Files & Spectral Simulations

5.1 Introduction

To make spectral calculations representative for several instruments, we need the response function (matrix) of a given instrument as an input in SPEX. The response function is given in the form of a binary response file `**.res` which defines the energy grid of the instrument, its spectral resolution, and the effective area. The binary spectrum `**.spo` file contains a dummy spectrum with a given exposure time and a background determined from a certain area (box) on the detector surface outside the region of the spectrum. Both the size of the background area and the exposure time can be changed during the session. See chapter 6 for more information about SPEX file formats.

5.2 Instruments

At the moment `**.res` and `**.spo` files are available for the following instruments:

- 1. EUVE
- 2. AXAF
- 3. XMM
- 4. SAX
- 5. ASCA
- 6. ...

The files are prepared in a fixed standard format and for each instrument a README file is available. With special programs we convert e.g FITS formatted files (available from instrumental groups) into SPEX readable files `**.res` and `**.spo`.

In the case of the EUVE spectrometers, where we do analyses on real data, we use the program EUVESPEX (and also SPEX) to generate specific `**.res` and `**.spo` files from the data of each individual observation.

In the documents, SRON/SPEX/TRIS01–05, we describe shortly the parameters of the instruments mentioned above such as spectral resolution, effective area and background. In the future more instruments can be added (e.g., *EINSTEIN* , *EXOSAT*, *ROSAT*, scanners of *EUVE*, Spectrum X-γ, etc.).

5.3 Spectral simulations

With SPEX, spectra can be generated using the instrumental files for several plasma models including statistical photon noise and background. Examples of various spectral simulations and analysis methods are given in the Cookbook (technical report SRON/SPEX/TRCB01).

Chapter 6

SPEX File Formats

6.1 Introduction

SPEX reads and writes the following file types:

- Spectral data (`*.spo` & `*.spa`)
- Response Matrices (`*.res` & `*.ras`)
- Energy grids (`*.egr`)
- DEM (Differential Emission Measure) files (`*.dem`)
- Other files : command (`*.com`), output (`*.out` & `*.asc`), PostScript (`*.ps` & `*.cps` & `*.vps` & `*.cvs`) and scratch files

The following sections will discuss the file format (i.e. the way in which data are written into a file) of each file type. Whenever possible, Fortran programs are presented that show how to create a specific file format.

6.2 Spectral data files

Spectral data are read or written in binary (`*.spo`) or ASCII (`*.spa`) format.

6.2.1 Writing spectral data in binary format (*.spo)

Binary files are opened as sequential, unformatted files and contain the following information (in designated order):

- Header

  A header consists of a number of header lines, with a maximum of 256 characters per line. The FIRST character of a header line **MUST** always be a `c` or a `C`!!! The rest of the headerline is arbitrary and may be used to provide the binary data file with relevant information about the data set itself, for example. The information in the header lines will be ignored by SPEX.

  The header **MUST** be closed by a line containing the following string: `SPEX`, `spex` or `Spex`. This indicates to SPEX that the header is finished and the following fields contain spectral data.

- nchan (`integer*4`), the number of output data channels. Should be smaller than or equal to nbmax (nbmax is currently set at 2048).

- TINTS(NBMAX) (`real*4` array), the total net integration time in s of the source spectrum as a function of bin number. Note that e.g. appending of spectra from other instruments to the current data set may lead to different integration times per channel.
- OCHAN(NBMAX) (`real*4` array), the observed spectrum in counts/s/bin.
- DOCHAN(NBMAX) (`real*4` array), the errors in the observed spectrum in counts/s/bin.
- BCHAN(NBMAX) (`real*4` array), the model background spectrum in counts/s/bin. This is used only for spectral simulations or for spectral fits where the expected instead of the observed number of counts is used in the weights of the fit statistic.
- FCHAN(NBMAX) (`real*4` array), the exposure ratio of the expected number of background counts in the source region to the expected number of background counts in the background region. Factors to be taken into account in this factor are e.g. exposure times, detector areas and average efficiencies of both parts. This array is only used for spectral simulations.

An example Fortran routine to write binary spectral data files is presented in Fig. 6.1.

6.2.2 Writing spectral data in ASCII format (*.spa)

ASCII files are opened as sequential, formatted files and contain the following information (in designated order):

- HEADER

  A header consists of a number of header lines, with a maximum of 256 characters per line. The FIRST character of a header line **MUST** always be a `c` or a `C`!!! The rest of the headerline is arbitrary and may be used to provide the binary data file with relevant information about the data set it self, for example. The information in the header lines will be ignored by SPEX.

  The header **MUST** be closed by a line containing the following string: `SPEX`, `spex` or `Spex`. This indicates to SPEX that the header is finished and the following fields contain spectral data.

- NCHAN (`integer*4`), the number of output data channels. Should be smaller than or equal to NBMAX (NBMAX is currently set at 2048).
- lines containing the following information:

  I TINTS(I) OCHAN(I) DOCHAN(I) BCHAN(I) FCHAN(I)

  where I ranges from 1 to NCHAN. The definition of the other data fields can be found in §6.2.1.

  NOTE: When SPEX reads an ASCII spectral data file, I is considered as a *dummy* variable. Therefore it is **important** that the sequence in which the data are written **originally**, is correct! Whenever a spectral data set is written in ASCII format from within the SPEX program, SPEX will of course use the correct value of I.

An example Fortran routine to write ASCII spectral data files is presented in Fig. 6.2.

```
        integer*4 nbmax
        parameter(nbmax=2048)
        integer*4 nchan
        real*4 tints(nbmax),ochan(nbmax),dochan(nbmax),bchan(nbmax),fchan(nbmax)
c
        .....
        .....
c
        open (unit=10,file='dummy.spo',status='unknown',
    &          access='sequential',form='unformatted')
        write (10) 'C This is the first header comment line'
        write (10) 'C You are allowe to have 0 comment lines in SPEX'
        write (10) 'C But always end the header with a line starting with SPEX'
c
        .....
        .....
c
        write (10) 'C This is the last header comment line'
        write (10) 'SPEX'
        write (10) nchan
        write (10) (tints(i),i=1,nchan)
        write (10) (ochan(i),i=1,nchan)
        write (10) (dochan(i),i=1,nchan)
        write (10) (bchan(i),i=1,nchan)
        write (10) (fchan(i),i=1,nchan)
        close(unit=10,status='keep')
        end
```

Figure 6.1: Example Fortran program to create binary spectral data files that are readable for SPEX.

6.3 Response Matrices

In SPEX, the response R(IC,IE) is defined as the number of expected counts in channel IC for 1 photon/m^2 in input energy bin number IE. Note that the effective detector area has been included in the response, it is **not** a free normalisation parameter! The effective detector area may contain sharp detector-edges. SPEX offers the possibility to define these edges in order to exclude the possibility of erroneous interpolation at these edges. SPEX then interpolates the edge correctly, starting at the correct side of the edge (if the response matrix is read in and **another** input energy grid has been defined than is included in the response file itself). It is always safer to include the edges as one of the input boundaries.

Response matrices may be read or written in binary (`*.res`) or ASCII (`*.ras`) format. Only data for which the response is non-zero are written! This optimizes the memory usage of SPEX. For this purpose *response groups* are defined. A response group is a sequence of consecutive channels for a fixed input bin number for which all response elements are non-zero. Note that in principle one input energy bin can consist of several response groups. Example: data for a grating where the higher orders

```
        integer*4 nbmax
        parameter(nbmax=2048)
        integer*4 nchan
        real*4 tints(nbmax),ochan(nbmax),dochan(nbmax),bchan(nbmax),fchan(nbmax)
c
        .....
        .....
c
        open (unit=10,file='dummy.spa',status='unknown',
    &          access='sequential',form='formatted')
        write (10,'(a)') 'C This is the first header comment line'
c
        .....
        .....
c
        write (10,'(a)') 'C This is the last header comment line'
        write (10,'(a)') 'SPEX'
        write (10,*) nchan
        do i = 1,nchan
          write (10,'(i5,5(1pg14.6))')
     &      i,tints(i),ochan(i),dochan(i),bchan(i),fchan(i)
        enddo
        close(unit=10,status='keep')
        end
```

Figure 6.2: Example Fortran program to create ASCII spectral data files that are readable for SPEX .

can form separate groups.

6.3.1 Writing response matrices in binary format (*.res)

Binary files are opened as sequential, unformatted files and contain the following information (in designated order):

- Header

  A header consists of a number of header lines, with a maximum of 256 characters per line. The FIRST character of a header line **MUST** always be a `c` or a `C`!!! The rest of the headerline is arbitrary and may be used to provide the binary data file with relevant information about the data set it self, for example. The information in the header lines will be ignored by SPEX.

  The header **MUST** be closed by a line containing the following string: `SPEX`, `spex` or `Spex`. This indicates to SPEX that the header is finished and the following fields contain spectral data.

- NCHAN (`integer*4`), the number of output data channels. Should be smaller than or equal to NBMAX (currently set at 2048).

- ECHAN1(NBMAX) (`real*4` array), the lower energy limits of the observed spectrum data channels in keV.
- ECHAN2(NBMAX) (`real*4` array), the upper energy limits of the observed spectrum data channels in keV.
- NEG (`integer*4`), the number of bins for the energy grid on which the spectrum is represented.
- EG1(NEMAX) (`real*4` array), the lower bin boundaries in keV for the energy grid on which the spectrum is represented.
- EG2(NEMAX) (`real*4` array), the upper bin boundaries in keV for the energy grid on which the spectrum is represented.
- NKRESP (`integer*4`), the total number of response groups. A response group is a continuous sequence of output channels for which the response matrix is positive, at a given input energy.
- KRESP(3,NCMAX) (`integer*2` array). The second argument corresponds to the response group number. For each response group, this array contains the following 3 quantities (stored as `integer*2`):
  1. The number of non-zero response elements of this group.
  2. The input energy bin number corresponding to this group.
  3. The output channel number for the first element of this group.
- NRESP (`integer*4`), the number of non-zero response matrix elements.
- RESP(NRESPMAX) (`real*4` array), the response matrix elements. Note that any effective area is already included in the response value: the RESP-value represents the expected number of counts/s in a certain output energy channel for 1 photon/s in the original energy bin. Although the response matrix is 2-dimensional, the array RESP is 1-dimensional and it contains compressed information: only non-zero response matrix elements are stored; indexing takes place via the array KRESP.
- NDETEDG (`integer*4`), the number of edges in the effective area of the instruments.

Only if NDETEDG > 0 then follows:

- EDETEDG(NDETEDGMAX) – real*4 array, the edges (in keV) in the effective area of the instrument. Needed for interpolations of the effective area.

An example Fortran routine to write binary response matrices is presented in Fig. 6.3.

6.3.2 Writing response matrices in ASCII format (*.ras)

ASCII files are opened as sequential, formatted files. The file content is the same as that of the binary files: first a header, then the data. For readability the data are written in the following designated order:

```
        integer*4 nbmax,nemax,ncmax,nrespmax,ndetedgmax
        parameter(nbmax=2048,nemax=8192,ncmax=32768,nrespmax=524288,
     &    ndetedgmax=64)
        integer*4 nchan,neg
        real*4 echan1(nbmax),echan2(nbmax),eg1(nemax),eg2(nemax)
        integer*2 kresp(3,ncmax)
        real*4 resp(nrespmax),edetedg(ndetedgmax)
c
        .....
        .....
c
        open (unit=10,file='dummy.res',status='unknown',
    &          access='sequential',form='unformatted')
        write (10) 'C This is the first header comment line'
        write (10) 'C You are allowe to have 0 comment lines in SPEX'
        write (10) 'C But always end the header with a line starting with SPEX'
c
        .....
        .....
c
        write (10) 'C This is the last header comment line'
        write (10) 'SPEX'
        write (10) nchan
        write (10) (echan1(i),i=1,nchan)
        write (10) (echan2(i),i=1,nchan)
        write (10) neg
        write (10) (eg1(i),i=1,neg)
        write (10) (eg2(i),i=1,neg)
        write (10) nkresp
        write (10) ((kresp(j,i),j=1,3),i=1,nkresp)
        write (10) nresp
        write (10) (resp(i),i=1,nresp)
        write (10) ndetedg
        if (ndetedg.gt.0) write (10) (edetedg(i),i=1,ndetedg)
        close(unit=10,status='keep')
        end
```

Figure 6.3: Example Fortran program to create binary response matrices that are readable for SPEX.

- HEADER

  A header consists of a number of header lines, with a maximum of 256 characters per line. The FIRST character of a header line **MUST** always be a `c` or a `C`!!! The rest of the headerline is arbitrary and may be used to provide the binary data file with relevant information about the data set it self, for example. The information in the header lines will be ignored by SPEX.

  The header **MUST** be closed by a line containing the following string: `SPEX`, `spex` or `Spex`. This indicates to SPEX that the header is finished and the following fields contain spectral data.

- NCHAN (`integer*4`), the number of output data channels. Should be smaller than or equal to NBMAX (NBMAX is currently set at 2048).

- lines containing the following information:

  I ECHAN1(I) ECHAN2(I)

  where I ranges from 1 to NEG. ECHAN1(I) and ECHAN2(I) are described in §6.3.1.

  NOTE: When SPEX reads an ASCII response matrix, I is considered as a *dummy* variable. Therefore it is **important** that the sequence in which the data are written **originally**, is correct! Whenever a response matrix is written in ASCII format from within the SPEX program, SPEX will of course use the correct value of I.

- NEG (`integer*4`), the number of bins for the energy grid on which the spectrum is represented.

- lines containing the following information:

  I EG1(I) EG2(I)

  where I ranges from 1 to NCHAN. EG1(I) and EG2(I) are described in §6.3.1. Remember to write the data in the right sequence!

- NKRESP (`integer*4`), the total number of response groups, and NRESP (`integer*4`), the total number of non-zero response elements. Both quantities should appear on the same line. A response group is a continuous sequence of output channels for which the response matrix is positive, at a given input energy.

- NKRESP response groups, containing the following information for group I:

  First line:

  KRESP(1,I) KRESP(2,I) KRESP(3,I)

  followed by RESP(*) for the KRESP(1,I) elements of the specific group. When SPEX writes an ASCII response matrix, per line 5 data fields will be written. This is however not mandatory for the input of an ASCII response matrix.

- NDETEDG (`integer*4`), the number of edges in the effective area of the instruments.

Only if NDETEDG > 0 then follows:

- lines containing EDETEDG(I), where I ranges from 1 to NDETEDG. When SPEX writes an ASCII response matrix, per line 5 data fields will be written. This is however not mandatory for the input of an ASCII response matrix.

An example Fortran routine to write ASCII response matrices is presented in Fig. 6.4.

```
        integer*4 nbmax,nemax,ncmax,nrespmax,ndetedgmax
        parameter(nbmax=2048,nemax=8192,ncmax=32768,nrespmax=524288,
     &    ndetedgmax=64)
        integer*4 nchan,neg
        real*4 echan1(nbmax),echan2(nbmax),eg1(nemax),eg2(nemax)
        integer*2 kresp(3,ncmax)
        real*4 resp(nrespmax),edetedg(ndetedgmax)
c
        .....
        .....
c
        open (unit=10,file='dummy.ras',status='unknown',
    &         access='sequential',form='formatted')
        write (10,'(a)') 'C This is the first header comment line'
c
        .....
        .....
c
        write (10,'(a)') 'C This is the last header comment line'
        write (10,'(a)') 'SPEX'
        write (10,*) nchan
        do i = 1,nchan
          write (10,'(i5,2(1pg14.6))') i,echan1(i),echan2(i)
        enddo
        write (10,*) neg
        do i = 1,neg
          write (10,'(i5,2(1pg14.6))') i,eg1(i),eg2(i)
        enddo
        write (10,*) nkresp,nresp
        k1 = 1
        k2 = 1
        do i = 1,nkresp
          write (10,'(3i5)') (kresp(j,i),j=1,3)
          k2 = k2 + kresp(1,i) - 1
          write (10,'(5(1pg14.6,:))') (resp(j),j=k1,k2)
          k2 = k2 + 1
          k1 = k2
        enddo
        write (10,'(i5)') ndetedg
        if (ndetedg.gt.0) write (10,'(5(1pg14.6,:))') (edetedg(i),i=1,ndetedg)
        close(unit=10,status='keep')
        end
```

Figure 6.4: Example Fortran program to create ASCII response matrices that are readable for SPEX.

6.3.3 Useful software

The example Fortran routine in Fig. 6.5 may be useful to convert a square SPEX matrix into a compressed form. In this example not only zero or negative response values are left out, but also response values that are negligably small (smaller than a user defined variable RLIM).

6.4 Energy grids (*.egr)

An input energy grid file is a simple ASCII-file containing one bin-border per line, starting with the lower limit from the first bin and ending with the upper limit from the last bin. The data should be ordered in ascending energy, and should be in units of keV.

An energy grid file with the following lines:

5

6

7

8

produces 3 bins: bin 1 from 5-6 keV, bin 2 from 6-7 keV and bin 3 from 7-8 keV.

Note: if data from various instruments are to be combined, it is best to save the instrument energy grids separately and merge them later on into a new file that can be sorted with the UNIX sort utility in ascending energy order.

6.5 DEM files (*.dem)

DEM files are ASCII files containing at most 8192 lines of data. Each line constists of 3 datafields:

- temperature (keV)
- differential emission measure (DEM) in $10^{64}/\mathrm{m}^3/\mathrm{keV}$
- error in the DEM

The DEM is defined as

$$\frac{n_\mathrm{e} n_\mathrm{H} \mathrm{d}V}{\mathrm{d}T}, \tag{6.1}$$

with n_e the electron density, n_H the Hydrogen density, V the volume and T the temperature.

When a DEM file is read, the error in the DEM is not read. However, when a DEM file is written the error is written as well.

```
      integer*4 nbmax,nemax,ncmax,nrespmax,ndetedgmax
      parameter(nbmax=2048,nemax=8192,ncmax=32768,nrespmax=524288,
     &    ndetedgmax=64)
      integer*4 nchan,neg
      real*4 echan1(nbmax),echan2(nbmax),eg1(nemax),eg2(nemax)
      integer*2 kresp(3,ncmax)
      real*4 resp(nrespmax),edetedg(ndetedgmax)
c
      real*4 r(nemax,nbmax),rlim
      parameter(rlim=.....)
c
      ......
      ......
c
      nresp = 0
      k     = 0
      do ie = 1,ne
        rprev = 0.
        do ic = 1,nchan
          if (r(ic,ie).gt.rlim) then
            nresp = nresp + 1
            resp(nresp) = r(ic,ie)
            if (rprev.le.rlim) then
              k          = k + 1
              kresp(1,k) = 0
              kresp(2,k) = ie
              kresp(3,k) = ic
            endif
            kresp(1,k) = kresp(1,k) + 1
          endif
          rprev = r(ic,ie)
        enddo
      enddo
      nkresp = k
      end
```

Figure 6.5: Example Fortran program to convert a square SPEX matrix into a compressed form.

Note: SPEX **interpolates** the DEM on a previously defined temperature grid (when setting the parameters of the DEM component). For a capricious DEM (e.g. with narrow peaks) inaccuracies might occur. Perhaps a newer version of SPEX can first integrate over the final DEM bin and then take the mean.

6.6 Other files

6.6.1 Log files (*.com)

SPEX provides options to 'record' and 'play back' SPEX commands using so called *log files*. A log file is a series of (previously recorded) SPEX commands that can be executed by SPEX again. To learn more about the log file structure, see chapter 7.

6.6.2 Output files (*.out)

Various types of output from SPEX may be stored into a file e.g. runtime output, data, model and parameter information etc. To learn more about the possibilities, see this manual §3.2.

6.6.3 ASCII output files (*.asc) from plasma model components

SPEX provides options to save plasma model properties into ASCII files. To learn more about these options, see this manual §3.8.

6.6.4 PostScript files

The graphical output from SPEX may be written to PostScript files. For this purpose, SPEX uses the PGPLOT interface. A typical PostScript file may contain several 'pages'. PGPLOT uses the standard Adobe convention, and the PostScript files may be printed or used for other purposes (e.g. encapsulating in documents). To learn more about the various types of PostScript files generated by SPEX, see this manual §3.8.

6.6.5 Scratch files

SPEX uses various temporary scratch-files. These files normally will be removed when the program is left. However, when SPEX is aborted or encounters a program crash, these scratch-files must be removed by hand. **NEVER** delete these temporary files when running SPEX!

Chapter 7

SPEX Log File Structure & Usage

7.1 Introduction

SPEX may be run in three different modes:

1. "classical" terminal mode
2. window mode
3. log file mode

When SPEX is run in mode 1 or 2, mode 3 may always be used.

SPEX provides options to 'record' and 'play back' SPEX commands using so-called *log files*. These log files are especially useful to be used as 'macros', to do 'routine' jobs such as setting models, reading data etc. A log file is an ASCII file and therefore it may easily be edited with any editor. In this way, useful sets of SPEX commands may be precompiled.

The following sections will describe in detail the principles of creating, recording and using these log files.

7.2 Log File Structure

A line in a log file may either contain a *command* or a *comment*.

7.2.1 Command lines

There are two types of command lines:

1. menu **ITEM**
2. menu **ITEM** *input*

'menu' is a menu acronym with a maximum of 4 characters; it should be unique. The index of document SRON/SPEX/TRUM03 contains all current menu acronyms (displayed in lowercase).

'**ITEM**' is a menu item. This is also an acronym with a maximum of 4 characters. Within each menu, all menu items have unique acronyms. Throughout the entire menu structure of the SPEX program, the menu item acronyms do not have to be unique. The index of document SRON/SPEX/TRUM03 contains all current menu item acronyms (displayed in uppercase).

'*input*' is an input field. Several types of data may be entered:

- an `integer*4` variable
- a `real*4` variable
- a character string with a maximum of 256 characters.

  Note: when the input field is used to enter a filename, only 252 characters can be used to specify the filename. 4 characters are needed to append the extension of the filename (this is done internally).

Some notes:

1. It may occur that several variables (`real*4` or `integer*4`) need to be entered at the same time. In those situations, SPEX reads the input as a character string (256 characters) and extracts the variables from the string.
2. 'menu' and '**ITEM**' need to be separated by at least one space. The same condition holds for '**ITEM**' and '*input*'.
3. It does not matter if 'menu' or '**ITEM**' are entered in either lower or upper case. SPEX will convert 'menu' to lower case and '**ITEM**' to upper case automatically. However, the case of the '*input*' field is very important. Whenever file names are entered through the '*input*' field, one should keep in mind that UNIX is case sensitive!

7.2.2 Comment lines

Comment lines may be added to the log file to explain certain steps in the log file. The first character of a comment line **must** be a # at the beginning of a new line! The comment line has a maximum of 256 characters. There is no restriction to the number of comment lines that follow each other in a log file.

It might be a good convention to put the comment line *before* a command line.

There are two ways to add comment lines to a log file:

1. After a certain part of a SPEX session is recorded and the log file is closed, comment lines may be added to the file.
2. At the SPEX command prompt, comment lines may be added to the log file that is used to store the commands of that particular session. The comment is entered by typing a # first, followed by the comment itself. Note that this is only possible when SPEX is actually storing commands to a log file (i.e. the log file must be open). Further, it is **not** possible to add a comment to the log file when SPEX requests specific numerical input.

7.3 Creating Log Files

Log files may be created in two ways:

1. by storing the commands during a SPEX session. See the user's manual §3.2 for more information about the options that SPEX offers.
2. by editing a new file with any ASCII editor. Note that this option is only recommended to experienced SPEX users!

In both cases the log file will have the extension `*.com`.

7.3.1 SPEX session recording

When log files are created by SPEX, only those commands are stored that do **not** refer to new menus. For example: the command 'MAIN' will not be stored. The same holds for a number of commands with which a user may go from one menu to another. By using the commands in a log file, SPEX can access a menu item directely.

There are however a few situations in which the intermediate steps are stored:

- When the menu item is '**COMP**', for the menus par, err, ste1, ste2, ste3, ste4, aspe & ptyp.
- When the menu item is '**PARA**', for the menus par, err, ste1, ste2, ste3 & ste4.

In these situations it is not obvious to SPEX from which menu the menu item was requested. For example:

'**COMP**'

may be used to select a new spectral model component or to select an already existing spectral model component for ASCII output. It then is beter to use:

par **COMP** comp **A02**

to select additive component 2 to modify one of it's parameters.

7.3.2 Manual composition

When log files are to be edited by hand, chapter 3 of the user's manual should be used to select the correct menu acronyms and menu item acronyms.

7.3.3 Nesting of Log Files

SPEX allows nesting of log files up to 20 levels deep. This means that log files may be executed from within log files. For example

....
exe **NAME** *filename*
exe **OPEN**
....

where *filename* is the explicit file name of the log file, **without** the extension `*.com` of course. After the line containing `exe OPEN` commands will follow that need to be executed after the execution of the commands in the log file named *filename*.

Note that whenever SPEX reads from one log file and, at the same time, writes to another log file, the commands that were read will not be stored again. In this situation, the same construction as presented above may be used.

7.4 Using Log Files

It is important to know that whenever log files are used to execute commands, the menus will not be displayed when SPEX is run in terminal mode.

Various examples of log files can be found in chapter 2 of this manual and in document SRON/-SPEX/TRCB01 .

7.4.1 Error handling

When SPEX encounters an error in a log file, the program will return immediately to the log file executing the specific log file. When the log file was executed from the interactive mode, SPEX will return to the interactive mode. In both situations, SPEX will report an error in the log file and all consecutive commands will be disregarded. SPEX returns to the menu that was called last by the log file.

When SPEX has executed a log file succesfully, this will be reported too and SPEX will return to the menu that was called last by the log file.

Appendix A

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