../doc/spurion.tex
created from help file
../help/spurion.hlp

May 14, 2002

Contents

Chapter 1

spurion

```
 SPURION- program to calculate spurious processes from ICP-like buffers
 or data files.

 To run on Jazz: "Jazz:~ % spur"
 To view documentation (html, latex, PS, PDF) based on the help files,
  www.ncnr.nist.gov/resources/spur
```

1.1 spurion:Version

```
This help file is spurion.hlp
 and associated documentation generated from this file is
../doc/spurion.tex
../doc/spurion/spurion.html
 documents the following version of SPURION:

  ************************************************************************
  * spur_020430_$(g77,sgi). V0.4.13 April, 2002. Used on 2002-04-30  11:39:1 *
  *                            Written by Jeff Lynn, the dark ages, ca. 1970 *
  *                       Graphical version written by Carl Adams, Feb. 2001 *
  *                       Modified by Tanya Riseman, Nov, 2001 - March, 2002 *
  ************************************************************************

Help file spurion.hlp last modified April 30, 2002 by Tanya Riseman.
```

1.2 spurion:Authors

```
SPURION was written by
```

```
  Jeff Lynn, the dark ages, ca. 1970   (original punch-card version)
  Carl Adams, 1997 - 2000 (graphics and Bragg Intensities)
NIST center for Neutron Research. Now at St. Xavier University.
  Tanya Riseman, 2001-2002 (debugging, Scan graphics, menus)
NIST center for Neutron Research. Ext 8379. Room E010.

The LAZY and PULVERIX subroutines was originally written by
   K. YVON, circa 1977-1989
   LABORATOIRE DE CRISTALLOGRAPHIE AUX RAYONS X
UNIVERSITY OF GENEVA
24 QUAI ERNEST ANSERMET, CH 1211 GENEVA, SWITZERLAND
TEL 022 219355
        ADAPTED TO B6700 AT UCSD, HANS F. BRAUN, 7 FEB. 1979
        ADAPTED TO CDC 7600 AT BNL, D. E. COX, DEC. 1984

modified  3.87 to prepare CPDF/PROFIL input file by P.ZOLLIKER

The HELP subroutine was written by
    Paul Kienzle, 1997
University of Birmingham
Birmingham, UK
```

1.3 spurion:Disclaimer

```
Although the SPURION program has been tested by its authors no
 warranty is made as to the accuracy and functioning.

Although the LAZY_PULVERIX has been extensively tested by its authors
 no warranty is made as to the accuracy and functioning.

The values of wavelengths, scattering factor constants and the
 equivalent positions used by the program are part of the output and the user
 is advised to compare them with the values given in the international tables
 for crystallography.
```

1.4 spurion:Help

```
  The help file spurion.hlp has a hierarchical tree structure.
 It is an ASCII file, based on the VMS help facility. The first column
 should be reserved for a number character (1-9), indicating the depth of the
 help topic. The name of the help topic follows the depth number.
 If the character in the first column is "!", the line is ignored as a comment.
```

```
 1. Type '?' to get a list of help topics at your current level.
 2. Type 'thistopic' to get the help for one of the help topics.
 3. Type 'thistopic subtopic subsubtopic' to skip down the tree quick,
    if you remember the path.
 4. Type carriage return to go up a help level. Eventually you will
    return to the calling program SPURION.
 5. You may truncate the help topic to the shortest unique set of characters.

The help routine needs the environment variable MSRHELP to be set in
 order to find the help file spurion.hlp, which is probably in the same
 directory as the source code. At the shell level, depending on the OS (VMS or
 Unix) and the UNIX shell being used:
 On VMS, "assign <helpdir> MSRHELP:"
 On Unix,"setenv MSRHELP <helpdir>" or "export MSRHELP='<helpdir>'"
```

1.5 spurion:PGPLOT

```
By now you should have two plots "pages" for a default scan:
 1. A "lattice" page of reciprocal space in the scattering plane of the
    spectrometer showing the Q, ki, and kf for the first and last points
    of the scan.
 2. A "scan" page showing the data (if the scan information is from a data file)
    and all the important spurions.
 If not, you may have problems with the PGPLOT environment variables.
 They are set in a script file (/usr/local/bin/spur on Jazz or runspurion_linux)
 that sets environment variables and then runs the SPURION program:

  On jazz.ncnr.nist.gov (OS is SGI):
(This is the up-to-date public version)
#! /bin/sh
 PGPLOT_DEV='/xserver'
 PGPLOT_ENVOPT='I'
 PGPLOT_XW_WIDTH='0.7'
 export PGPLOT_DEV  PGPLOT_ENVOPT PGPLOT_XW_WIDTH
 PGPLOT_DIR='/usr/user2/cpadams/pgplot/'
 PGPLOT_FONT=' /usr/user2/cpadams/pgplot/grfont.dat'
 MSRHELP='/usr/local/lib/spur'
 export PGPLOT_DIR PGPLOT_FONT MSRHELP
/usr/local/bin/spur.bin

On a Linux machine such as Tanya Riseman's desktop computer:
(This is the current development version)
 PGPLOT_DEV='/xserver'
 PGPLOT_ENVOPT='I'
 PGPLOT_XW_WIDTH='0.7'
```

```
 export PGPLOT_DEV  PGPLOT_ENVOPT PGPLOT_XW_WIDTH
 PGPLOT_DIR='/usr/local/share/pgplot/'
 PGPLOT_FONT='/usr/local/share/pgplot/grfont.dat'
 MSRHELP='/home/tanya/for/spuriondir/src_0204/'
 export PGPLOT_DIR PGPLOT_FONT MSRHELP
 /home/tanya/for/spuriondir/bin/spur_020430_g77

If you are porting or modifying SPURION, you may get copies of the
 the PGPLOT library and documentation from the official PGPLOT web site:
 http://www.astro.caltech.edu/~tjp/pgplot/
```

1.6 spurion:Overview

```
By now you should have two plots "pages" for a default scan:
 1. A "lattice" page of reciprocal space in the scattering plane of the
    spectrometer showing the Q, ki, and kf for the first and last points
    of the scan.
 2. A "scan" page showing the higher order spurions energies vs.scan point.

  Using the command "dm", you may read in scattering information from
 a q-buffer (<base>.buf) or from the header of a data file (<base>.bt*) to
 replace the default values that the q-buffer variables are initialized with.
 Information about the crystal structure and the Bragg peak intensities
 are inferred from a Lazy-Pulverix input file (<base>.lpi) that you can enter
 with the command "dm". The default is a square lattice and no information
 about the Bragg intensities, which is the case when the Lazy-Pulverix
 information is missing.
```

1.7 spurion:Lattice_plot

```
In the "lattice" plot, the inner and outer shaded area represents
 regions of reciprocal space that cannot be accessed for 0<A4<115 degrees with
 any pairs of |ki| and |kf| in the scan.  The inner dashed circles are the
 A4=0,115 boundaries for the least favorable ki-kf pairs.  Some information
 about  the scan is also given along with calculated values of the reciprocal
 lattice units for the zeta and eta directions in inverse Angstroms.  There may
 be  some reduction of the given orientation vectors which prevents SPURION
 from  skipping reciprocal lattice points (??Huh??).

 If a lazy-Pulverix file (<base>.lpi) has been read in, the "lattice"
 plot will show the structure and indicate which peaks are strong, weak and
 (optionally) absent.  Consult this help file under INPUTFILES command for
 information about the LPI files.  The Sf(Q=0)^2 value is shown and should be
```

```
equal to the sum of scattering lengths in the unit cell squared.  Sfq^2 values
and systematic absences are calculated with no Lorentz or thermal factors.
Look at the output file <base>.struct if you wish to verify that the generated
atoms are in the  correct positions in the unit cell. If there are errors when
reading the LPI file, you can find diagnostic information in the file
<base>.log.
```

1.8 spurion:Scan_plot

```
The "scan" plot shows has two basic plots:
 1. The experimental intensity vs scan point (if a data file *.bt* was used)
    with the positions of likely spurions optionally super-imposed.
    In the case of those higher order spurions which intercept Bragg peaks, the
    Sf^2 of the Bragg peak is used a relative "intensity" for the spurion.
      a. Higher order spurions are yellow.
      b. Elastic spurions are red
      c. Aluminum spurions from the sample holder are green.
      d. Incoherent spurions from the monochromator/analyzer are cyan/blue.
 2. The energy of the higher order spurions vs. scan point.
    Higher order spurions which intersect Bragg peaks are indicated in yellow.
    Elastic spurions (dE = 0) are in red.

Both horizontal axes are in terms of the "scan" point, that is,
 the sequential order of the scan. If the scan is a temperature scan,
 a temperature axes will appear on the top of the top most plot.
 Between the two plots, the  angle A4 appears, and perhaps the
 Q values and/or the energies of the scan is either of them vary.
```

1.9 spurion:MainMenu

```
Summary of SPURION program main menu commands.
```

1.9.1 spurion:MainMenu:MENUsnapshot

```
   The first line is the executable's name, version number and today's date.

   The second line is where serious warnings appear, related to
 inconsistencies in the q-buffer. This warning line also appears in red on
 both the "lattice" page and the "scan" page.
```

```
   The third line are the input files which have been successfully read in.

   Each row of the menu has a 2 character option command, a description,
 a logical indicating if the option is in use, a logical
 indicating if the option is the one most recently selected and a short string
 indicating what numerical values are in use related to the option.
 The two logicals should not be needed by the user.

Snap shot of main menu:
Command ("q" to quit)?
 spur_020430_$(g77,sgi). V0.4.13 April, 2002. Used on 2002-04-30  11:39:19

SPUR_DEFAULT.buf          SPUR_DEFAULT.lpi                SPUR_DEFAULT.<ext>
 dm: Start over with defaults or new files             F F S
 s : Toggle plot higher-order scattering spurions      F F
 i : Toggle plot incoherent scattering spurions        T F mon=    0 ana=    0
 a : Toggle plot aluminum Ewald spheres                F F
 o : Toggle plot u and v orientation vectors           F F nabsent=    0/    0
 l : Toggle label Q, Ki and Kf wavevectors             F F
 g : Toggle overlay grid on lattice plot               T F o: 1.000 1.000
 mm: Modify Q, E, and other Q-buffer values            F F
 t : Change the rlv, energy spurion tolerances         F F  0.050 A^-1 1.00 meV
 b : BUMP! change maximum A4                           F F   115.00     degs
 f : Sf^2 for an (hkl) reflection                      F F ( 0, 0, 0)=  0.0
 z : Zoom spurion energy plot (0,0,0,0 for auto)       F F   0   0   0.0   0.0
 r : Rescale plot (reverse xmin and xmax for left)     F F  Right handed spectm
 sm: Presentation of structure factors menu            F F
 n : Toggle display of notes next to plot              T T
 pw: Printout/ change graphics device                  F F
 bw: Write out Q-buffer to a file                      F F  no bufout yet
 gw: Generate spectrometer angles-ICP dry run          F F  no icp yet
 h : HELP!!                                            T F
 QQ: to quit                                           F F
Command ("QQ" to quit)? h
```

1.9.2 spurion:MainMenu:dm_DefaultMenu

```
 dm: Start over with defaults or new files

The "dm" command allows you to read in new q-buffer information from
 either a q-buffer (<base>.buf) or from a data file (<base>.bt#), or continue
 to use the current q-buffer values in memory, or start all over with the
 program's default values.  This is the purpose of the first question in the
 dialog.  Next, you may optionally select lazy-Pulverix  information which
 defaults to none used, the current selected file,  a new file with the same
 base name as the q-buffer or data file (<base>.lpi) or a file with an
```

```
 arbitrary name.

The output file names are automatically based on the q-buffer name
 (<base>.buf) or data file read in (<base>.bt#). If no file is read in,
 the base name becomes <base> = "SPUR_DEFAULT".
```

1.9.2.1 spurion:MainMenu:dm_DefaultMenu:Inputfiles

```
  Input file names will be of the form
        <base>.buf   (Q buffer from experiment)
     or <base>.bt#   (ICP triple axis data file, #= 0 - 9)
     <base>.lpi      (Lazy Pulverix input file, optional)

    For more information about the q-buffer file, see the help topic
 "Inputfiles BUF".

    For more information about the data file, see the help topic
 "inputfiles BT".

    For more information about the LPI file, see the help topic
 "inputfiles LPI".
```

1.9.2.2 spurion:MainMenu:dm_DefaultMenu:Outputfiles

```
  Output file names will be of the form
     <base>.struct   (Structure information)
     <base>.spur     (Spurion information)
     <base>.log      (Log file, in case program fails)
     <base>.debug    (Temporary debugging info)

  Optional output file names will be of the form
     <base>.bufout   (Optional output Q buffer from this program)
     <base>.icp      (Optional ICP dry run, contains spect angles)
     <base>_bw.ps    (Optional B&W postscript file, lattice plot)
     <base>_cl.ps    (Optional color postscript file, lattice plot)
     <base>_scbw.ps  (Optional B&W postscript file, scan plot)
     <base>_sccl.ps  (Optional color postscript file, scan plot)

The output file names are automatically based on the q-buffer name
 (<base>.buf) or data file read in (<base>.bt#). If no file is read in,
 the base name becomes <base> = "SPUR_DEFAULT".
```

1.9.2.3 spurion:MainMenu:dm_DefaultMenu:Dialog

```
Dialog:
What sort of q-buf info do you want to input?
 d:   default values set by program
 c:   current values in program
 b:   q buffer file              <base>.buf
 0-9: ICP triple axis data file  <base>.bt#
 h:   HELP!!
Enter q-buf choice (d,c,b,0-9, h):  b

What sort of q-buf info do you want to input?
 d:   default values set by program
 c:   current values in program
 b:   q buffer file              <base>.buf
 0-9: ICP triple axis data file  <base>.bt#
 h:   HELP!!
Enter q-buf choice (d,c,b,0-9, h): b
```

1.9.3 spurion:MainMenu:s_Spurion

```
 s : Toggle plot higher-order scattering spurions

SPURION will calculate the Q-positions of scattering processes
 resulting from n*ki-m*kf where n and m range from 1 to 4.  These spurions
 correspond to higher order reflections from the monochromator and analyzer.

 On the "Lattice" page:
 The higher order spurions are shown with yellow and red dots.  Red dots
 correspond to elastic scattering (dE = 0) and yellow inelastic on the
 "Lattice" page. Any spurions that match non-absent Bragg reflections are
 shown with arrows. Consider the amount of higher-order scattering from
 monochromator and analyzer, the E of the spurious process, and the relative
 Bragg peak intensity which contributes the spurious process.  The match to
 the Bragg reflections is governed by the spatial tolerance factor, which you
 can change with the "t" command. The elastic scattering has dE=0 to within
 the energy tolerance, which you can also change with the "t" command.

On the "Scan" page:
 Those higher order spurions which match within q-tolerances of a Bragg peak
 are indicated by yellow symbols on the "Scan" page. The intensity plotted is
 proportional the the Sf^2 of the Bragg peak on the top plot, if Bragg peak
 intensities are available. The bottom plot
 shows the energy of the higher order spurions vs. scan point.

All elastic spurions and those inelastic spurions which are within
```

tolerance of Bragg peaks are written to the screen. All spurions are written out to the output file <base>.spur.

1.9.4 spurion:MainMenu:i_Incoherent

i: Toggle plot incoherent scattering spurions

??? Check colors in code!

SPURION will calculate the Q-positions of scattering processes ki-|ki|*kf/|kf| and |kf|*ki/|ki|-kf. These are processes where the scattering from the sample is elastic and either the monochromator or analyzer is scattering incoherently but with directions governed by A3 and A4. (Imagine you are using vanadium as a MON or ANA. Not such a smart idea!) Shown with cyan dots or blue dots with arrows if it matches a non-absent Bragg peak. Spurions are written to <base>.spur. The amount of incoherent scattering from MON and ANA and the relative Bragg peak intensity determine the strength of this spurious process. This process can be verified experimentally by changing A1 or A5 with A2 or A6 held constant. In addition, I know that I have performed experiments with Si MON/ANA Xtals and Al powder scattering at the sample contributed to this process. Check this manually by the positions of Al Ewald spheres relative to the cyan dots. The matching of Bragg reflections is governed by the q-tolerance factor, which you can change with the t command.

On the "Scan" page:
Those incoherent spurions which match within q-tolerances of a Bragg peak are indicated by cyan symbols for the monochromator and blue symbols for the analyzer on the top plot of the "Scan" page.

1.9.5 spurion:MainMenu:a_Aluminum

a : Toggle plot aluminum Ewald spheres

SPURION calculates the Al Ewald spheres and compares their radii in reciprocal space to |Q|. The spheres are plotted in green or in red if it matches a Q in the scan.
The matching is controlled by the tolerance factor which may be changed by the t command. Any spurions are saved in <base>.spur. Aluminum is face-centered cubic so only h,k,l all even or all odd reflections will be present and the calculation uses lattice parameter a=4.04096 A.

On the "Scan" page:
Those aluminum spurions which match within q-tolerances of a scan point Q

are indicated by green symbols on the "Scan" page.

1.9.6 spurion:MainMenu:o_Orientation

o : Toggle plot u and v orientation vectors

The orientation vectors, whose (hkl) are given in the axes labels, are plotted in magenta.

Bug: the arrowhead size is often too large.

1.9.7 spurion:MainMenu:l_Labelwave

l : Toggle label Q, Ki and Kf wavevectors

Label the ki, -kf, and Q wave vectors and state the energy transfer. You can either overwrite the plot (blotting out the graphics below) or just overlay the labels.

Carl Adams: I have done my best to try and get the labels in sensible places with reasonable sizes but what you see is what you get. Let me know what kind of problems you encounter.

1.9.8 spurion:MainMenu:g_Grid

g : Toggle overlay grid on lattice plot

Plots a dashed line grid over the reciprocal lattice plot on the "LATTICE" page, with your choice of u- and v- step size give in rlu's. You have the choice of the grid being Cartesian-style or using the u and v orientation vectors.

1.9.9 spurion:MainMenu:mm_ModifyMenu

mm : Modify Q, E, and other Q-buffer values

One of the most powerful SPURION commands. With the "mm" command you can nearly any of the q-buffer parameters in memory, thereby modifying the

```
 scan conditions of the q-buffer and see how the spurions are affected.  The
 modifications do not take effect until you exit this sub-menu.  Note: any
 inconsistent modifications should produce warnings and  errors, including
 bright red warnings on the bottom of the plots and at the top of the main
 menu.  There are no guarantees that all possible inconsistencies will be
 caught.  However, most errors should be correctable by reentering this modify
 menu.

Summary of modify sub-menu commands.
```

1.9.9.1 spurion:MainMenu:mm_ModifyMenu:MENUsnapshot

```
   The first line is a description of the sub-menu.

   The second line are the input files which have been successfully read in.

   Each row of the menu has a 2 character option command, a description,
 a logical indicating if the option is in use, a logical
 indicating if the option is the one most recently selected and a short string
 indicating what numerical values are in use related to the option.
 The two logicals should not be needed by the user.

Snap shot of the modify sub-menu:
 Modify buffer parameters.
SPUR_DEFAULT.buf          SPUR_DEFAULT.lpi              SPUR_DEFAULT.<ext.>
 lp: Lattice: parameters a, b, c                       F F  3.14  3.14  3.14 A
 la: Lattice: angles aa, bb, cc                        F F  90.0  90.0  90.0 Dg
 ec: Energy: at center of scan                         F F   0. meV
 es: Energy: step                                      F F   1. meV
 fe: Energy: value of fixed (MON) or (ANA)             F F   14.6999998 meV
 mo: Energy: toggle MON or ANA with E-fixed            F F  (ANA) is fixed
 dm: Energy: lattice spacing of MON                    F F   3.35400009 A
 da: Energy: lattice spacing of ANA                    F F   3.35400009 A
 qc: Space: qh qk ql at center of scan                 F F (1.10,1.10,0.00)
 qs: Space: qh qk ql step                              F F (0.00,0.00,0.00)
 u : Orient: u=(hkl) of scattering plane               F F (   1,   1,   0)
 v : Orient: v=(hkl)' of scattering plane              F F (   0,   0,   1)
 t0: Temp/H: start temperature T0                      F F   300. K
 ts: Temp/H: temperature step inc-T                    F F   0. K
 np: Time: number of scanned (E,Q,T) points            F F  5
 h : HELP!!                                            F F
 q : to quit                                           F F
Command ("q" to quit)?
```

1.9.9.2 spurion:MainMenu:mm_ModifyMenu:lp_latticeparms

```
lp: Lattice: parameters a, b, c
```

1.9.9.3 spurion:MainMenu:mm_ModifyMenu:la_latticeangles

```
la: Lattice: angles aa, bb, cc
```

1.9.9.4 spurion:MainMenu:mm_ModifyMenu:ec_energycenter

```
ec: Energy: at center of scan
```

1.9.9.5 spurion:MainMenu:mm_ModifyMenu:es_energystep

```
es: Energy: step
```

1.9.9.6 spurion:MainMenu:mm_ModifyMenu:fe_fixedenergy

```
fe: Energy: value of fixed (MON) or (ANA)
```

1.9.9.7 spurion:MainMenu:mm_ModifyMenu:mo_MonOrAnaFixed

```
mo: Energy: toggle MON or ANA with E-fixed

 Either the monitor or the analyzer has fixed energy.
This command toggles which one is fixed.
```

1.9.9.8 spurion:MainMenu:mm_ModifyMenu:dm_lattcSpacingMON

```
dm: Energy: lattice spacing of MON
```

1.9.9.9 spurion:MainMenu:mm_ModifyMenu:da_lattcSpacingANA

```
da: Energy: lattice spacing of ANA
```

1.9.9.10 spurion:MainMenu:mm_ModifyMenu:qc_qcenter

```
qc: Space: qh qk ql at center of scan
```

1.9.9.11 spurion:MainMenu:mm_ModifyMenu:qs_qstep

```
qs: Space: qh qk ql step
```

1.9.9.12 spurion:MainMenu:mm_ModifyMenu:u_uScatteringPlane

```
u : Orient: u=(hkl) of scattering plane
```

1.9.9.13 spurion:MainMenu:mm_ModifyMenu:v_vScatteringPlane

```
v : Orient: v=(hkl)' of scattering plane
```

1.9.9.14 spurion:MainMenu:mm_ModifyMenu:t0_tempStart

```
t0: Temp/H: start temperature T0
```

1.9.9.15 spurion:MainMenu:mm_ModifyMenu:ts_tempStep

```
ts: Temp/H: temperature step inc-T
```

1.9.9.16 spurion:MainMenu:mm_ModifyMenu:np_pntsInScan

```
np: Time: number of scanned (E,Q,T) points
```

1.9.9.17 spurion:MainMenu:mm_ModifyMenu:h_Help

```
h : HELP!!
```

1.9.9.18 spurion:MainMenu:mm_ModifyMenu:q_Quit

```
q : to quit sub-menu
```

1.9.10 spurion:MainMenu:t_Tolerance

```
t : change the tolerance for spurions

Change the q and energy tolerance factors used in the "s" higher order
 spurions, "i" incoherent spurions, and "a" aluminum spurion calculations.
 The user should keep in mind what the instrumental resolution really is,
 and modify the values accordingly. Ideally, eventually this program will
 automatically calculate reasonable resolutions. Currently the program uses
 either 0.05 AA_1 or the q step size for the q tolerance and
 either 1 meV or the energy step size for the energy tolerance.

 Dialog:
 Current rlv tolerance 0.050 AA^-1.  Enter new value. 0.05
 Current energy  tolerance 1.000 meV?.  Enter new value. 1.
```

1.9.11 spurion:MainMenu:b_bump

```
b : BUMP! change maximum A4

  Change the maximum for the spectrometer's angle A4. Defaults to
 115 degrees.
```

1.9.12 spurion:MainMenu:f_Flection

```
 f : Sfq^2 for an (hkl) reflection in the scattering plane

Given that the intensity scaling of the reflections is quite rough use
 the f command to give Sfq^2 directly.  No Lorentz or thermal factors are
 included.  At present only those Sfq^2 which are in scattering plane can be
 calculated. The value is printed to screen and also appears in the
 "notations" section of the "lattice" plot and on the main menu.
 If the requested h,k,l is accidentally not in the scattering plane, a list of
 the possible q values is printed out.

     While SPURION is in the testing phase pay close attention to the
 atomic positions and scattering lengths given in <base>.struct when comparing
 this value of Sfq^2 to those given by other programs or procedures.  Inform
 Tanya Riseman or Carl Adams of discrepancies.
```

1.9.13 spurion:MainMenu:z_ZoomScanPlots

```
 z : Zoom spurion energy plot (0,0,0,0 for auto)

   On the "lattice" page, select horizontal range for scan points
 (min=0, max=# of scanpoints) and the vertical range for the higher order
 spurions' energies. Enter xmin_npts, xmax_npts, ymin_e, ymax_e
 separated by spaces or commas. Use zeros to have the program use the
 full range by default.
```

1.9.14 spurion:MainMenu:r_rescaleLattcPlot

```
 r : rescale plot (reverse xmin and xmax for left)

At the prompt enter xmin,xmax,ymin,ymax separated by spaces or commas.

You may switch to a left-handed coordinate system and spectrometer by
 making xmin larger than xmax.
```

1.9.15 spurion:MainMenu:sm_StrucFactorMenu

```
 sm: Presentation of structure factors sub-menu
```

```
Modify the presentation of the reciprocal lattice plot on the "LATTICE"
 page. Note: If no lazy-Pulverix input file (*.lpi) is being used, this
 sub-menu is of no use.

Summary of structure factors sub-menu commands.
```

1.9.15.1 spurion:MainMenu:sm_StrucFactorMenu:MENUsnapshot

```
   The first line is a description of the sub-menu.

   The second line are the input files which have been successfully read in.

   Each row of the menu has a 2 character option command, a description,
 a logical indicating if the option is true/false, a logical
 indicating if the option is the one most recently selected and a short string
 indicating what numerical values are in use related to the option.
 The two logicals should not be needed by the user.
 The first logical is used to remember the presentation options.

Snap shot of the structure factors sub-menu:
 Modify display of Bragg intensities
ceb.buf                    ceb.lpi                                  ceb.<ext.>
 s : Toggle display Bragg intensities                  T F  Sf^2 not shown
 n : Toggle rep. intensities by circles/numbers        F F  circles
 c : Toggle rep. intensities by color/grey scale       T T  color
 z : Rel. circle size                                  F F   1.
 u : Toggle circle size uniform or vary with Sf^2      F F  uniform
 l : Toggle show/hide sorting labels                   F F  ABC..cba labels
 a : Toggle display/hide systematic absences           F F  hide absences
 g : Toggle  bunching sort by S^2= base^n or +- tol    F F  sort by +- tol
 t : Select sorting tolerance (+- tol)                 F F      0.007     = tol
 b : Select sorting base: (base^(n-1) < S^2 < base^n   F F
 h : HELP!!                                            F F
 q : to quit                                           F F
```

1.9.15.2 spurion:MainMenu:sm_StrucFactorMenu:s_DisplaySf

```
 s : Toggle display Bragg intensities

  Can stop displaying the Bragg peak intensities Sf^2 as
 if there was no lazy- Pulverix input file.
```

1.9.15.3 spurion:MainMenu:sm_StrucFactorMenu:n_NumbersOrCircles

```
 n : Toggle rep. intensities by circles/numbers

Label the Bragg peak intensities Sf^2 on the Lattice plot
 by either numbers or by circles.
```

1.9.15.4 spurion:MainMenu:sm_StrucFactorMenu:c_colorOrGrey

```
 c : Toggle rep. intensities by color/grey scale

Represent the relative intensity by either a grey scale
 or a blue-green color scale. Affects both circles and numbers.
```

1.9.15.5 spurion:MainMenu:sm_StrucFactorMenu:z_circleSize

```
 z : Rel. circle size

  A scaling factor for the size of the circles plotted.
 1 is the default size. Greater than 1 makes larger circles.
 Only affects circles, not numbers.
```

1.9.15.6 spurion:MainMenu:sm_StrucFactorMenu:u_uniformCircles

```
 u : Toggle circle size uniform or vary with Sf^2

Circles can be draw with a uniform size or with their radii
 proportional to the Bragg peak's intensity. Only affects circles, not numbers.
```

1.9.15.7 spurion:MainMenu:sm_StrucFactorMenu:l_sortingLabels

```
 l : Toggle show/hide sorting labels

The intensity values are sorted. They are optionally
 noted in a key on the right hand size of the page if the
 main menu item "n" notations is selected. The individual intensities
 are optionally labeled on the plot by a code 'ABC...cba"
 with the largest intensity labeled by "A" and the smallest by "a".
 This command toggles whether the labels are shown on the plot.
```

1.9.15.8 spurion:MainMenu:sm_StrucFactorMenu:a_absences

```
a : Toggle display/hide systematic absences

 Systematic absences are optionally marked off by green crosses.
```

1.9.15.9 spurion:MainMenu:sm_StrucFactorMenu:g_logSorting

```
g : Toggle  bunching sort by S^2= base^n or +- tol

 Different Bragg peaks will have the same intensities SF^2, such as
(1,0,1) and (1,0,-1). However, Lazy-Pulverix does not return exactly the
same values. We want to label intensities which are nearly the same
by the same label. Therefore, we sort the intensities, and those
which are within tolerance (+- tol) of each other are deemed to be identical.
This is called the "linear" sorting scheme.

 This command toggles between the default sorting scheme described above
and one based on a log scale, base b. The log-sorting scheme bunches all
intensities which are between base^n and base^(n+1) and gives those
intensities a common label. This is useful when there are many
different intensities and one wants to quickly identify those which are large
or small quickly. This is called the logarithmic sorting scheme.
```

1.9.15.10 spurion:MainMenu:sm_StrucFactorMenu:t_sortingTol

```
t : Select sorting tolerance (+- tol)

 This is only used  when using a normal "linear" sorting scheme
has been selected. See the help option g_logSorting (for command "g").
```

1.9.15.11 spurion:MainMenu:sm_StrucFactorMenu:b_sortingBase

```
b : Select sorting base: (base^(n-1) < S^2 < base^n

 This is only used  when using a "logarithmic" sorting scheme
has been selected. See the help option g_logSorting (for command "g").
```

1.9.15.12 spurion:MainMenu:sm_StrucFactorMenu:h_help

```
 h : HELP!!
```

1.9.15.13 spurion:MainMenu:sm_StrucFactorMenu:q_quit

```
 q : to quit sub-menu
```

1.9.16 spurion:MainMenu:n_Notations

```
 n : Toggle display of notations next to plot

Notations are optionally placed on the "Lattice" and (eventually)
 the "Scan" pages. Notations include
 1. q-buffer information, shown on the "Lattice" page.
 2. Which important main menu items have been selected, shown on the
    "Lattice" page.
 3. The labels and intensity circles (grey or colored) for the Bragg peak
    intensities, shown on the "Lattice" page.
    What is shown will depend on selections made in the "sm"
    sub-menu (presentation of structure factors).
```

1.9.17 spurion:MainMenu:pw_Printout

```
 pw: printout/change graphics device

 This is the printout command.  You can change the graphics device from
 the default X-server to either black and white postscript or color
 postscript for either the "lattice" page or the "scan" page.
 The generated PS file have a name based on the q-buffer or data file's name.

 Unfortunately, PGPLOT can only process one PS file at a time,
 so you must ask for both the "lattice" and the "scan" pages separately.
 Currently, you can run other commands after this "pw" command, and they will
 appear in the PS file. Consequently you MUST close the PS file by either
 selecting another "pw" device number (like 0=XSERVE) or by quiting the program.
 Otherwise, the PS file will not be properly ended.
```

```
  If using gray scale, remember that for the white on black X-window,
 white is most intense but for black on white postscript black is most intense.
 Colors will come out as black on back and white printers.

 dialog:
 Device #   =0 for XSERVE (screen, no printout)
            =1 for XWIN (screen, no printout)
            =2 for B&W postscript file: <base>_bw.ps   = lattice plot
            =3 for color postscript file: <base>_cl.ps   = lattice plot
            =4 for B&W postscript file: <base>_scbw.ps = scan plot
            =5 for color postscript file: <base>_sccl.ps = scan plot
  Apologies: PGPLOT can only process one PS "window" at a time.
  To properly close a PS file, a new device must be selected or quit program.
Enter device number (0-5)
```

1.9.18 spurion:MainMenu:bw_qbufferWrite

```
 bw: Write out Q-buffer to a file

  Outputs the q-buffer variables to <base>.bufout, in same format as
input q-buffers *.buf.
```

1.9.19 spurion:MainMenu:gw_Genangles

```
 gw: generate spectrometer angles

Another powerful calculational command that reproduces the dry run of
 ICP. Outputs to <base>.icp.

 Tanya: I can change the formating of <base>.icp to assist it s usage as input
 to another program, if desired.

 Carl Adams:  While SPURION is still in the testing phase it probably makes
 sense to confirm that it agrees with ICP (at least within 0.005 degrees).
 If there are discrepancies contact Tanya Riseman or Carl Adams ASAP
 and we will fix the problem.  DO NOT BELIEVE the output of SPURION if it does
 not agree with ICP!!  I have included a few things in SPURION to check the
 validity of the buffer with warnings when appropriate but it may miss things
 that ICP does not.

 Matt Woodward: The numbers look OK.
```

1.9.20 spurion:MainMenu:h_Help

```
 h : HELP!!

Give either a general help/description of SPURION or give details of
 SPURION commands.  Reproduced in the file spurion.hlp

Details of the behavior of the help() routine:

  The help file spurion.hlp has a hierarchical tree structure.
 It is an ASCII file, based on the VMS help facility. The first column
 should be reserved for a number character (1-9), indicating the depth of the
 help topic.

Type '?' to get a list of help topics at your current level.

Type 'thistopic' to get the help for a one of the help topics.

Type 'thistopic subtopic subsubtopic' to skip down the tree quick,
 if you remember the path.

Type carriage return to go up a help level. Eventually you will
 return to the calling program SPURION.

  You may truncate the help topic to the shortest unique set of
 characters.
```

1.9.21 spurion:MainMenu:q_Quit

```
 q : to quit


Remember that the output files are may be overwritten if the same
 base file name is reused, so rename them if you have result you would like
 to keep them.
```

1.10 spurion:Background

```
This help section discusses background information.
```

1.10.1 spurion:Background:Spectrometer

1.10.2 spurion:Background:Bragg

1.11 spurion:Inputfiles

```
  Input file names will be of the form
      <base>.buf      (Q buffer from experiment)
      <base>.lpi      (Lazy Pulverix input file)
```

1.11.1 spurion:Inputfiles:BT

```
     <base>.bt#   (ICP triple axis data file, #=0-9)
 Works for BT2 presently.

*** Expand ************** ????
```

1.11.1.1 spurion:Inputfiles:BT:example

The header portion of a data file (pross007.bt2):

```
'PROSS007.BT2' '12-AUG-2001 12:43' 'Q'    1175000.    6  'NEUT'  105  'RAW'
  Filename         Date            Scan       Mon    Prf  Base   #pts  Type
PrOsS  PrOs4Sb12                                 =20
 60 20 40  2       0  0  0         1  0  0   0.000     0  0  1
 Collimation        Mosaic              Xstal Orientation
     6.283     6.283     6.283    90.000    90.000    90.000
Lattice Parameters in real space
    11.000    -0.250       14.700        3.354   3.354      6.00000   0.00000
    E center  Delta E      EA fixed      M-dsp   A-dsp     Tmp strt   Tmp inc
  1.800   0.000   0.000    0.0000  0.0000  0.0000      0.0000
   Q (hkl scan center)        Delta Q (hkl)            Hfield
    Q(x)    Q(y)    Q(z)     E       T-act    min       Counts
  1.8000  0.0000  0.0000  24.0000  8.00510    5.95          21
```

```
  1.8000  0.0000  0.0000  23.7500  8.02280    5.97          26
...
  1.8000  0.0000  0.0000  -2.0000  7.90630    6.36          12
```

1.11.2 spurion:Inputfiles:BUF

```
This section describes the required format of a input q-buffer file.
*** Expand ************** ???

The program is now better at being able to read in <base>.buf files
 which have had spaces removed or added in the course of hand editing.
 (Hopefully no editing will be necessary after the file created using
 cut-and paste between windows).  The overall ICP format is required,
 particularly the colons ":" and equal signs "=" after labels.
```

1.11.2.1 spurion:Inputfiles:BUF:example

```
 Qbuffer No:  3   Comment: EuMnP  Xtal
 Lattice:  a: 4.1396  b: 4.1396  c: 4.1396  aa: 90.000  bb: 90.000  cc:90.000
 Energy:  EC: 5.0000 ES: 1.000 FE: 14.700 (ANA)  dM= 3.3542  dA= 3.3542
 Space:   HC: 1.0000 KC: 1.0000 LC: 0.0000  HS: 0.0000  KS: 0.0000  LS: 0.0000
 Orient:  (h k l): 1, 1, 0  Angl:  0.000    (h k l)': 0, 0, 1
 Temp/H:  T0:1.2000  Inc-T.00000  Wait:  0  Err:.50  Hld0:  0  Hld:  0  Field
 Time:    Monit: 110000  Prefac:  1  M-typ:TIME  #pts:   11   AMON    POLA FKEY
```

1.11.3 spurion:Inputfiles:LPI

```
This section describes the required format of a lazy PULVERIX
 input file LPI.

The original lazy-PULVERIX has rather strict fixed format requirements
 for the LPI. We have relaxed them, so that the output from the WWW application
 Lazy can be read, plus additional relaxations so that hand editing is not so
 dangerous. The input of the LPI file is now case insensitive.  Where there is
 free formating reads allowed, parameters may be separated by spaces, commas or
 tabs. Blank parameters are indicated by a comma, e.g. ' ,'.

  Only the first 2 characters of each command are inspected,
 but the read routines expect all the characters to be present, followed by a
 space, then followed by the command's parameters.

Adapted from http://barns.ill.fr/dif/icsd/lazy_reference.html
```

1.11.3.1 spurion:Inputfiles:LPI:Title

```
Sample title (Required)

The title is the remainder of the line after the first 6 characters 'TITLE '
Include for example the chemical formula and diffraction conditions. This
title will be used to label the plot.
```

1.11.3.2 spurion:Inputfiles:LPI:COndit

```
Experimental conditions (Optional)

The CONDIT line is NOT essential.

example: CONDIT CUA1 1.59460 3 80.0 N 2GN N

FORMAT(3A2,4X,  A4,     F8, F3, F5, 1X,A1, I2,    A2,   1X,A1)
       'CONDIT', SYMWL, WL, TL, TH,  NORM, IMAGE, SYMLP, IANO
```

1.11.3.2.1 spurion:Inputfiles:LPI:COndit:CONDIT

```
Columns 1- 6  CONDIT    PUNCH CARD LABEL  *CONDIT*
```

1.11.3.2.2 spurion:Inputfiles:LPI:COndit:SYMWL

```
Columns  11-14  SYMWL     SYMBOL FOR WAVELENGTH
                          ADJUST TO THE LEFT OF THE FIELD.
                          EXAMPLE
                          CUA1 = COPPER K ALPHA1 RADIATION.
                          THE LIST OF ALLOWED SYMBOLS IS GIVEN AT
                          THE END OF THIS DESCRIPTION.
                          WAVELENGTHS FOR WHICH NO SYMBOL EXIST
                          MUST BE GIVEN EXPLICITLY IN COLS 15-20.
                          IF LEFT BLANK CU K ALPHA RADIATION IS
                                                  ASSUMED.
                          NEUTRON DIFFRACTION
                          LEAVE COLUMNS 11-14 BLANK AND GIVE
                          VALUE OF WAVELENGTH IN COLUMNS 15-20.

Example:  CUA1 is the characteristic wavelength symbol Cu-Ka1.
```

1.11.3.2.3 spurion:Inputfiles:LPI:COndit:WL

```
   Columns  15-20  WL        WAVELENGTH IN ANGSTROM
                              NEED NOT BE GIVEN IF SYMWL IS SPECIFIED

   Example:  1.5946 is the wavelength value - only needed if CUA1 blank.
  If no value is given, CUA1 is assumed.

 W A V E L E N G T H S    (VARIABLE *SYMWL* ON CONDIT CARD)

  THE LINES CONTAIN THE SYMBOLS FOR K ALPHA1, K ALPHA2 AND
  THE WEIGHTED AVERAGE OF THE K ALPHA RADIATION FOR CHROMIUM, IRON,
  COPPER, MOLYBDENUM AND SILVER.
  THE WAVELENGTHS IN ANGSTROM ARE GIVEN IN PARENTHESES

  CRA1 (2.28970)    CRA2 (2.29361)    CR (2.2909)
  FEA1 (1.93604)    FEA2 (1.93998)    FE (1.9373)
  CUA1 (1.54056)    CUA2 (1.54439)    CU (1.5418)
  MOA1 (0.70930)    MOA2 (0.71359)    MO (0.7107)
  AGA1 (0.55941)    AGA2 (0.56380)    AG (0.5608)
```

1.11.3.2.4 spurion:Inputfiles:LPI:COndit:TL

```
   Columns  21-25  TL        LOWER THETA -LIMIT OF CALCULATION

   Example:  3 is the minimum theta angle. If blank, 0.0 is assumed.
```

1.11.3.2.5 spurion:Inputfiles:LPI:COndit:TH

```
   Columns  26-30  TH        UPPER THETA -LIMIT OF CALCULATION
                             IF LEFT BLANK  TL=0 AND TH=89 DEGREES.
                             FOR GUINIER CAMERAS TH IS 45 DEGREES

   Example:  80.0 is the maximum theta angle. If blank, 89.0 is assumed.
  (or 45.0 for Guinier cameras).
```

1.11.3.2.6 spurion:Inputfiles:LPI:COndit:NORM

```
   Columns     32  NORM      TABULAR REPRESENTATION OF THE POWDER PATTERN.
                             BLANK   INTENSITIES NORMALIZED TO 1000
                             A       INTENSITIES NOT NORMALIZED
                             N       NO TABULAR REPRESENTATION OF
```

```
                                    THE POWDER PATTERN

 Example:  N means no tabular listing of the pattern,
blank means normalize strongest line to 10000,
and A means no normalization.
```

1.11.3.2.7 spurion:Inputfiles:LPI:COndit:IMAGE

```
 Columns  33-34  IMAGE     GRAPHIC REPRESENTATION OF THE POWDER PATTERN.
                           BLANK    NO GRAPHIC OUTPUT
                           INTEGER  GRAPHIC OUTPUT OF INTENSITIES
                                    IN STEPS OF 1/(2*INTEGER) OF
                                    THETA

 Example:  2 means listing in steps of 1/(2*2) degrees theta,
while blank means no listing.
```

1.11.3.2.8 spurion:Inputfiles:LPI:COndit:SYMLP

```
 Columns  35-36  SYMLP     EXPERIMENTAL TECHNIQUE
                           DS    DEBYE-SCHERRER
                           BLANK POWDER-DIFFRACTOMETER & MONOCHROMATOR
                           NE    NEUTRON DIFFRACTION
                           GN    GUINIER-DE WOLFF CAMERA
                           GH    GUINIER-HAEGG CAMERA
                                 THE FORMULAE FOR THE LORENTZ -
                                 POLARISATION FACTORS ARE GIVEN
                                 AT THE END OF THIS DESCRIPTION.
                            1    NO LP-FACTOR CORRECTION APPLIED

 Example:  GN represents the diffraction technique, where:
BLANK means Debye-Scherrer or diffractometer data.
NE means NEutron powder diffractometer.
GN means GuiNier camera.
GH means Guinier-Hagg camera.
1 means no Lorentz polarization correction.
(Lorentz polarization factors given later).
```

1.11.3.2.9 spurion:Inputfiles:LPI:COndit:IANO

```
  Columns    38  IANO      CORRECTION FOR ANOMALOUS DISPERSION (X RAYS ONLY)
                           BLANK   CORRECTION IS MADE
```

```
                              N       NO CORRECTION IS MADE.

   Example:  N means no correction for anomalous dispersion.
  blank means dispersion correction.
  For ionized atoms (not recommended) no dispersion
  correction will be made, and no correction will
  be made for neutron, synchrotron (yet) nor other
  diffractometer data.
```

1.11.3.2.10 spurion:Inputfiles:LPI:COndit:notes

```
It is recommended to compute all structures with neutral atoms. If
 form factors for ionized atoms are used the programme will not make
 dispersion corrections.  No dispersion correction will be made for neutron
 diffraction.

If no CONDIT card is given, copper radiation and Debye-Scherrer
technique is assumed, correction for anomalous dispersion will be made and a
complete powder pattern will be calculated.
```

1.11.3.2.11 spurion:Inputfiles:LPI:COndit:lorentz

```
 Lorentz polarization factors (SYMLP)

 Debye-Scherrer technique
 L =  1.0/(sin(theta)**2*cos(theta))
 P = (1.0+ cos(2*theta)**2)/2.

 Guinier technique
 L =  1.0/(sin(theta)**2*cos(theta)*cos(2*theta-beta))
 P = (1.0+ cos(2*theta)**2*cos(2*alpha)**2)/(1+cos(2*alpha)**2)
 alpha = diffraction angle of monochromator.
 beta  = angle between the normal to the specimen and the
direction of the incident beam.

Note: alpha and beta depend on the geometry of the Guinier camera and
 the d-spacing of the reflecting planes of the monochromator crystal. For
 Guinier cameras other than Guinier-de Wolff or Guinier-Hagg, or for
 monochromator crystals other than quartz, changes in the programme have to be
 made.
```

1.11.3.3 spurion:Inputfiles:LPI:CEll

```
  Lattice constants  (Required)

 example: CELL 4.5678, 5.6789 16.7890, 90 122.3, 90

 Free format (separated by spaces, tabs or commas)
'CELL', A, B*, C*, Alpha*, Beta*, Gamma*

 Note: Items (*) which may be left blank, must use a comma to indicated
 that the item is blank unless they are at the end of the line. See help items
 below for the situations in which items may be left out.

A, B, and C are lattice parameters in angstroms.

Alpha, Beta, Gamma are the lattice angles in degrees.
```

1.11.3.3.1 spurion:Inputfiles:LPI:CEll:Cubic

```
  Omit B,C,ALPHA,BETA,GAMMA
```

1.11.3.3.2 spurion:Inputfiles:LPI:CEll:Hexagonal

```
 Omit B,ALPHA,BETA, and set GAMMA=120.
```

1.11.3.3.3 spurion:Inputfiles:LPI:CEll:Rhombohedra

```
  Rhombohedral cells should be calculated on Hexagonal axes.
 If Rhombohedral axes are required, the structure must be described in the
 Triclinic system.
```

1.11.3.3.4 spurion:Inputfiles:LPI:CEll:Tetragonal

```
 Omit B,ALPHA,BETA,GAMMA
```

1.11.3.3.5 spurion:Inputfiles:LPI:CEll:Orthorhombic

```
 Omit ALPHA,BETA,GAMMA
```

1.11.3.3.6 spurion:Inputfiles:LPI:CEll:Monoclinic

```
  Omit ALPHA,GAMMA
```

1.11.3.4 spurion:Inputfiles:LPI:SPcgr

```
  Space group (Required unless LAtice and SYmtry are used.)

  Free format

 example: SPCGRP P M N A

 example: SPCGRP P 21/C

The list of permitted symbols is given below, sorted by the lattice
 symmetry. No other symbols are permitted. Do NOT include the * preceding some
 of the symbols. The * indicates centrosymmetric space groups which have been
 described with several settings. The programme generates only the setting with
 the centre of symmetry at the origin of the unit cell. Note that instead of
 using the SPCGRP symbol, you may use the explicit space group operators. For
 non-standard settings, LATICE  and SYMTRY lines must be used.
```

1.11.3.4.1 spurion:Inputfiles:LPI:SPcgr:rules

```
  Hermann Mauguin symbol for the space group adjust to the left of the field.

 Rules for coding:

 * Symmetry operators are separated by a slash or by a blank.
 * The bar operation is coded as minus *-*.
 * Screw axes are given by two integers that are not separated by a blank.

 EXAMPLES:
  P B C N
P 21/C
P -3
```

1.11.3.4.2 spurion:Inputfiles:LPI:SPcgr:warning

```
For all other symbols the programme may generate wrong equipoints
without error messages. Please check the listing  after running the programme.
For non standard space group settings SYMTRY- AND LATICE- cards must be used.
```

1.11.3.4.3 spurion:Inputfiles:LPI:SPcgr:notes

```
For centro-symmetric groups, the programme assumes the setting
 with the centre at the origin.

For R-space groups, the hexagonal setting is assumed R-space
 groups with rhombohedral axes must be simulated using LATICE and SYMTRY
 lines corresponding to a triclinic description.

Do NOT include the * preceding some of the symbols. The * indicates
 centrosymmetric space groups which have been described with several settings.
 The programme generates only the setting with the centre of symmetry at the
 origin of the unit cell. Note that instead of using the SPCGRP symbol, you may
 use the explicit space group operators (SYMTRY command).
```

1.11.3.4.4 spurion:Inputfiles:LPI:SPcgr:TRICLINIC

```
 P 1          P -1
```

1.11.3.4.5 spurion:Inputfiles:LPI:SPcgr:MONOCLINIC

```
 P 2          P 21         C 2          P M          P C
 C M          C C          P 2/M        P 21/M       C 2/M
 P 2/C        P 21/C       C 2/C

 The equivalent positions generated from these symbols correspond
 to the monoclinic setting with the b-axis unique (alpha=gamma=90)
```

1.11.3.4.6 spurion:Inputfiles:LPI:SPcgr:ORTHORHOMBIC

```
 P 2 2 2      P 2 2 21     P 21 21 2    P 21 21 21   C 2 2 21
 C 2 2 2      F 2 2 2      I 2 2 2      I 21 21 21   P M M 2
 P M C 21     P C C 2      P M A 2      P C A 21     P N C 2
 P M N 21     P B A 2      P N A 21     P N N 2      C M M 2
 C M C 21     C C C 2      A M M 2      A B M 2      A M A 2
 A B A 2      F M M 2      F D D 2      I M M 2      I B A 2
 I M A 2      P M M M     *P N N N      P C C M     *P B A N
 P M M A      P N N A      P M N A      P C C A      P B A M
 P C C N      P B C M      P N N M     *P M M N      P B C N
 P B C A      P N M A      C M C M      C M C A      C M M M
 C C C M      C M M A     *C C C A      F M M M     *F D D D
 I M M M      I B A M      I B C A      I M M A

Do NOT include the * preceding some of the symbols.
```

1.11.3.4.7 spurion:Inputfiles:LPI:SPcgr:TETRAGONAL

```
  P 4          P 41         P 42         P 43         I 4
  I 41         P -4         I -4         P 4/M        P 42/M
 *P 4/N       *P 42/N       I 4/M       *I 41/A       P 4 2 2
  P 4 21 2     P 41 2 2     P 41 21 2    P 42 2 2     P 42 21 2
  P 43 2 2     P 43 21 2    I 4 2 2      I 41 2 2     P 4 M M
  P 4 B M      P 42 C M     P 42 N M     P 4 C C      P 4 N C
  P 42 M C     P 42 B C     I 4 M M      I 4 C M      I 41 M D
  I 41 C D     P -4 2 M     P -4 2 C     P -4 21 M    P -4 21 C
  I -4 M 2     P -4 C 2     P -4 B 2     P -4 N 2     P -4 M 2
  I -4 C 2     P -4 2 M     I -4 2 D     P 4/M M M    P 4/M C C
 *P 4/N B M   *P 4/N N C    P 4/M B M    P 4/M N C   *P 4/N M M
 *P 4/N C C    P 42/M M C   P 42/M C M  *P 42/N B C  *P 42/N N M
  P 42/M B C   P 42/M N M  *P 42/N M C  *P 42/N C M   I 4/M M M
  I 4/M C M   *I 41/A M D  *I 41/A C D
```

Do NOT include the * preceding some of the symbols.

1.11.3.4.8 spurion:Inputfiles:LPI:SPcgr:TRIGONAL

```
  P 3          P 31         P 32         R 3          P -3
  R -3         P 3 1 2      P 3 2 1      P 31 1 2     P 31 2 1
  P 32 1 2     P 32 2 1     R 3 2        P 3 M 1      P 3 1 M
  P 3 C 1      P 3 1 C      R 3 M        R 3 C        P -3 1 M
  P -3 1 C     P -3 M 1     P -3 C 1     R -3 M       R -3 C
```

Note: All R-space groups refer to the hexagonal setting.

1.11.3.4.9 spurion:Inputfiles:LPI:SPcgr:RHOMBOHEDRAL

Rhombohedral cells should be calculated on Hexagonal axes. If Rhombohedral axes are required, the structure must be described in the Triclinic system.

1.11.3.4.10 spurion:Inputfiles:LPI:SPcgr:HEXAGONAL

```
  P 6          P 61         P 65         P 62         P 64
  P 63         P -6         P 6/M        P 63/M       P 6 2 2
  P 61 2 2     P 65 2 2     P 62 2 2     P 64 2 2     P 63 2 2
  P 6 M M      P 6 C C      P 63 C M     P 63 M C     P -6 M 2
  P -6 C 2     P -6 2 M     P -6 2 C     P 6/M M M    P 6/M C C
```

```
  P 63/M C M   P 63/M M C
```

1.11.3.4.11 spurion:Inputfiles:LPI:SPcgr:CUBIC

```
  P 2 3        F 2 3        I 2 3        P 21 3       I 21 3
  P M 3       *P N 3        F M 3       *F D 3        I M 3
  P A 3        I A 3        P 4 3 2      P 42 3 2     F 4 3 2
  F 41 3 2     I 4 3 2      P 43 3 2     P 41 3 2     I 41 3 2
  P -4 3 M     F -4 3 M     I -4 3 M     P -4 3 N     F -4 3 C
  I -4 3 D     P M 3 M     *P N 3 N      P M 3 N     *P N 3 M
  F M 3 M      F M 3 C     *F D 3 M     *F D 3 C      I M 3 M
  I A 3 D
```

Do NOT include the * preceding some of the symbols.

1.11.3.5 spurion:Inputfiles:LPI:ATom

```
  Atom identifier and coordinates (Required)

  Free format
'ATOM ' ELEMT, IDE*, X, Y, Z, BTEMP*, FOCCU*

 Note: Items (*) which may be left blank, must use a comma to indicated
 that the item is blank unless they are at the end of the line. See help items
 below for the situations in which items may be left out.

 example: ATOM CA 3 0.3333 0.6667-0.512 0.5 1.0

 example: ATOM CA 3 1/3,2/3,0.512 1/2 1

 example: ATOM CA2+ 4 1/3,2/3,0.512 1/2 1
```

1.11.3.5.1 spurion:Inputfiles:LPI:ATom:ELEMT

```
     Symbol of element and ionisation state.

  Only listed symbols listed an be given.

  Examples:
   CA   symbol for calcium(neutral)
CA2+ symbol for calcium(ionized)
```

Do NOT include the asterisk preceding an atom symbol. This asterisk indicates atom identifiers that are allowed for both X-ray and neutron

```
 diffraction.

All other symbols are allowed for X-ray diffraction only.

Atom symbols followed by a point have a special meaning (see below).

In case of X-ray diffraction, use neutral atoms unless you know exactly
 what you want to calculate.
```

1.11.3.5.1.1 spurion:Inputfiles:LPI:ATom:ELEMT:Symbols

```
 *AC    *C     *DY    *HE     LU3+   NP4+  *PU     SI.    TM3+
  AC3+   C.     DY3+  *HF    *MG     NP6+   PU3+   SI4+  *U
 *AG    *CA     ....   HF4+   MG2+   ....   PU4+   SM     U3+
  AG1+   CA2+  *ER    *HG    *MN    *O      PU6+   SM3+   U4+
  AG2+  *CD     ER3+   HG1+   MN2+   O1-    ....  *SN     U6+
 *AL     CD2+  *EU     HG2+   MN3+   O2-.   RA     SN2+   ....
  AL3+  *CE     EU2+  *HO     MN4+  *OS     RA2+   SN4+  *V
  AM     CE3+   EU3+   HO3+  *MO     OS4+  *RB    *SR     V2+
 *AR     CE4+   ....   ....   MO3+   ....   RB1+   SR2+   V3+
 *AS     CF    *F      I      MO5+  *P     *RE     ....   V5+
  AT    *CL     F1-    I1-    MO6+   PA    *RH    *TA     ....
 *AU     CL1-  *FE    *IN     ....  *PB     RH3+   TA5+  *W
  AU1+   CM     FE2+   IN3+  *N      PB2+   RH4+  *TB     W6+
  AU3+  *CO     FE3+  *IR    *NA     PB4+   RN     TB3+   ....
  ....   CO2+   FR     IR3+   NA1+  *PD    *RU    *TC    *XE
 *B      CO3+   ....   IR4+  *NB     PD2+   RU3+  *TE     ....
 *BA    *CR    *GA     ....   NB3+   PD4+   RU4+  *TH    *Y
  BA2+   CR2+   GA3+  *K      NB5+   PM     ....   TH4+   Y3+
 *BE     CR3+  *GD     K1+   *ND     PM3+  *S     *TI    *YB
  BE2+  *CS     GD3+   KR     ND3+   PO    *SB     TI2+   YB2+
 *BI     CS1+  *GE     ....  *NE    *PR     SB3+   TI3+   YB3+
  BI3+  *CU     GE4+  *LA    *NI     PR3+   SB5+   TI4+   ....
  BI5+   CU1+   ....   LA3+   NI2+   PR4+  *SC    *TL    *ZN
  BK     CU2+  *H     *LI     NI3+  *PT     SC3+   TL1+  *ZN2+
 *BR     ....   H.     LI1+  *NP     PT2+  *SE     TL3+  *ZR
  BR1-   D.     H1-   *LU     NP3+   PT4+  *SI    *TM     ZR4+
```

1.11.3.5.1.2 spurion:Inputfiles:LPI:ATom:ELEMT:Special

```
 Symbols with special meaning (indicated by a point '.'):
   H. hydrogen HF scattering factor
   C. carbon HF scattering factor
   SI. silicon HF scattering factor
```

```
   D. deuterium HF scattering factor
   O2-. taken from Acta Cryst. Vol.19, P.486(1965)
```

1.11.3.5.2 spurion:Inputfiles:LPI:ATom:IDE

```
Sequence number or atom label. (May be left blank.)
```

1.11.3.5.3 spurion:Inputfiles:LPI:ATom:XYZ

```
 X, Y, or Z coordinate.

Only coordinates between -1.and+1. are allowed.
 Fractions may be given as integers separated by a slash

 example:
ATOM   H    1/3     2/3    0.512
is equivalent to
ATOM   H    .33333 .666667 0.512
```

1.11.3.5.4 spurion:Inputfiles:LPI:ATom:BTEMP

```
 Debye-Waller factor

If left blank no temperature factor correction will be made.
```

1.11.3.5.5 spurion:Inputfiles:LPI:ATom:FOCCOU

```
 Occupation factor

This factor is usually 1 (=full occupancy of the site) but it may be
 smaller in disordered structures. If left blank full occupancy will be
 assumed.
```

1.11.3.6 spurion:Inputfiles:LPI:LAtice

```
  Optional

 FORMAT(3A2,2X,A1,2X,A1)
        'LATICE ' ISYMCE, SYMBR
 example: LATICE A P
```

```
 ISYMCE   CENTER OF SYMMETRY AT ORIGIN
          C   YES (CENTRIC) A   NO (ACENTRIC)

 SYMBR    BRAVAIS LATTICE INDICATOR
  P   PRIMITIVE       A   A CENTERED
  I   BODY CENTERED B   B CENTERED
  R   RHOMBOHEDRAL C   C CENTERED
  F   FACE CENTERED BLANK   PRIMITIVE

  * For Trigonal P-space groups, use P with the hexagonal setting.
  * For R-space groups, use R with an hexagonal cell (the programme assumes
    the standard obverse setting) or use P with a rhombohedral cell and give
    a, b, c and all angles on the cell card.
  * If no SPCGRP nor LATICE line is given, a primitive acentric cell is assumed.
```

1.11.3.7 spurion:Inputfiles:LPI:SYmtry

```
  Optional (but requited if SYMTRY lines are given).

  free format

 example: SYMTRY X, 1/2-Y, 1/2+Z

 Equivalent positions line is in free format with x,y,z separated by
 commas.

For centrosymmetric cells (ISYMCE=C in LATICE), give only one of the
 two centro-symmetrically related positions.

For I-, R-, F-, A-, B- and C- cells (SYMBR=I,R,F,A,B OR C in LATICE),
 give only one of the positions related by centering.

If no SYMTRY command is given, X,Y,Z is automatically assumed, however
 if SYMTRY commands are given then the X,Y,Z position must be included.

You may use the Bilbao Space Group Generator to obtain these space
 group generators (see http://www.cryst.ehu.es/cryst/get_gen.html).
```

1.11.3.8 spurion:Inputfiles:LPI:ENd

```
  Required

  END (This must be the last line for each structure set).
```

1.11.3.9 spurion:Inputfiles:LPI:FInish

```
  Required (but a bit redundant, since only do 1 material.)

Note: This command must come after the last end command.
 It initiates execution of the programme.
```

1.11.3.10 spurion:Inputfiles:LPI:example

```
TITLE  CeB6
CONDIT        1.55               NE
CELL         4.1396
SPCGRP    p m -3 m
atom   CE 1     0               0       0       0
ATOM   B,  ,    0.1993, 1/2,    1/2,     ,      0.94
END
FINISH
```

1.12 spurion:Outputfiles

```
  Output file names will be of the form
     <base>.struct   (Structure information, based on Lazy-Pulverix)
     <base>.spur     (Spurion information)
     <base>.log      (Log file, in case program fails)
     <base>.debug    (Temporary debugging info)

  Optional output file names will be of the form
     <base>.bufout   (Optional output Q buffer from this program)
     <base>.icp      (Optional ICP dry run, contains spect angles)
     <base>_bw.ps    (Optional B&W postscript file, lattice plot)
     <base>_cl.ps    (Optional color postscript file, lattice plot)
     <base>_scbw.ps  (Optional B&W postscript file, scan plot)
     <base>_sccl.ps  (Optional color postscript file, scan plot)
```

1.13 spurion:Warnings

```
Terse warnings appear on the second line of the main menu and also
```

```
appear in red on both the "lattice" page and the "scan" page.
Currently there are 4 separate kinds of warnings, nearly all of which
are due to logical inconsistencies in the values in the q-buffer in
memory, either as it was read in originally or subsequently modified.
 1. The scattering q is out of the scattering plane
    or the scattering triangle can not be closed
    or there is some problem with with calculating k_f.
 2. There is no item in the q-buffer which is stepped in the scan.
    Normally, either q, the energy or the temperature is stepped.
 3. The number of steps in the scan is either zero or larger than the
    array sizes in the program.
 4. Miscellaneous other warnings, involving nonsensical lattice angles and
    lattice parameters, or data files producing read errors.
```