NAME

LauePlot2.1, lp2.1 - plot histograms of crystallographic or any column-by-column data

SYNOPSIS

LauePlot2.1 or lp2.1 file1 [file2 ...] [-0 [divided-by]] [-1 [binx biny]] [-adhjrstuw] [-c i j] [-i [crystal]] [-l label] [-o [output1 output2 ...]] [-CDOSX size] [+a] [+p [ch ck cl]] [+u [ch ck cl]]

DESCRIPTION

The program LauePlot2.1 or lp2.1 plots 1- and 2-dimensional histograms of any column-by-column data file. Especially, the program plots crystallographic histograms since it can calculate the resolution of diffraction data from the Miller indices h, k, l columns.

OPTIONS

file1 [file2 ...]
: Free format input filename(s). Data must be organized in columns and no characters will be accepted.

[-0 [divided-by]]
: If division happens to have a value divided by zero, the program will set to 9999.0 by default. To change the default, choose this flag and specify the value you want to set. If this flag is chosen but nothing is specified, 0 is the second default.

[-1 [binx biny]]
: Plot 1-dimensional histograms. Binx and biny are the bin numbers for the horizontal and vertical axis. The default values are 30 and 20 respectively.

[+a]
: Turn on anomalous scattering difference, which means that the reflections (h k l) and (-h -k -l) will be treated as different reflections.

[-a]
: Accept all data when the error code column indicates some rejection. This option must work with -r option.

[-c i j]
: I, j are the column # of the input file(s). The first histogram will plot these two columns. The horizontal axis is column i, and the vertical axis is column j. I, j must be integers.

[-d]
: No graphical display. This is useful when the program is started from a non-sgi-graphical-window.

[-h]
: Print this manual pages.

[-i [crystal]]
: Xtal_info file crystal.xtl will be loaded in from current directory

or $CRYSTALINFO. Xtal_info is neccessary when the program calculates resolution from h, k, l values. If no crystal name is supplied, the program will use the environment value $CRYSTALNAME.

[-j]

Leave out rejected data when output. This option is always on when no error code is written. It makes difference only when the program is processing a data file with error code. And it only works when the -o option is selected.

[-l label]

Labels will be loaded from the file label, which has the following format:

```
lin h
lin k
lin l
... ...
res resolution (A)
lin wavelength (A)
log intensity
log sigma(I)
ope 13 / 14 or opl 13 / 14
opr 1 2 3
err error code or use error code
12 13 14 11 15 8 16 17 1 27 28 21 7 6 31 30
```

Each record specifies a label and a scale type of the column. Lin, res, log specifiy linear, reciprocal cubic, and logarithmic scale respectively; err or use indicates that this column is a 32 bits error code which can appear only at the last column of the file(s). Err and use are set and unset error code respectively. The numbers in the last record of the file are the bit numbers of the error code for each columns. In the above example, h, k, l, resolution, wavelength, intensity, sigma(I), I/sigma(I) and resolution calculated from hkl occupy the error bit number 12, 13, 14, 28, 21, 7, 6, 31 and 30 respectively. An implied column of arithmetic operation of 2 real columns (except error code column) could be added right before the error code column if any. Ope indicates such a column. The label of the implied column should be in the format of (column1) (arithmetic operator +, -, *, / and **) (column2). Opl indicates that the implied column is in logarithmic scale. Opr indicates an implied resolution column (in reciprocal cubic scale). The 3 numbers following are the column numbers of h, k, l. The -i option must be used at the same time if opr is in the label file. Implied column can also has an error bit.

[-o [output1 ...]]

Filename(s) of output data. If -o option has no filename followed, the program will ask for filenames and the output condition. This feature can be used to seperate an input file or to rearrange the input files.

[+p [ch ck cl]]

Prefix prime hkl columns on each record when output.

[-r]

Data rejection. The data file must have less than 32 columns with this option on. Bit 0 of the error code set means that this record is rejected, otherwise it is accepted. Bit n (n=1,...,31) set means that the value in column col, where n=bit(col), is out of selected range. But this does not mean that this record is rejected. Bit 0 could be the bit-OR of some bits n.

[-s]
No scratch file. With this option on, the program will not creat a scratch file for temporary data storage. This option is not recommanded when the data file is large since it slows down the data io.

[-t]
The program will ask for a title which will be printed on the histogram.

[+u [ch ck cl]]
Prefix LaueView unique hkl columns on each record when output. This option is useful when one wants to sort the data file in a symmetry related order using unix sort command. This option is working only when the other options -o and -i are functioning, otherwize it's ignored and/or working incorrectly. Ch ck cl are 3 integers which indicate the column numbers of h, k, l. If these numbers are not supplied, the program takes the default values 1, 2, 3.

[-u]
Ignore the first 13 characters of each record. This option will let the program load in a prefixed data file as same as loading a normal file. Then on output, it becomes normal.

[-w]
White background.

[-CDOSX size]
Select a symbol of a data point. Circle, dot, open square, solid square, and cross are selected respectively. Size is the size of the symbol, integer, > or = 0. If size < 0, it will be set to 0. The default is X 1. When you have a lot of data points, X 0 would be good choice. When you are plotting a curve, D 5 is OK.

EXAMPLES
The command line,

LauePlot2.1 ly01.sht -l sht.lab -c 13 14 +u -ro tmp.sht -i lyso -X 0

display histograms of data set ly01, reject some data and output to a temporary file tmp.sht with unique hkl prefix. The first histogram will be column 13 on the horizontal axis and 14 on the vertical. Xtal_info like cell parameters and space group symmetry will be loaded in from lyso.xtl. And each data point will ploted as a 1-pixel dot.

FILES
$LAUEVIEWHOME/man/laueplot.man, $LAUEVIEWHOME/lib/symmlib, ./$CRYSTALNAME.xtl, ./crystalname.xtl, $CRYSTALINFO/$CRYSTALNAME.xtl, $CRYSTALINFO/crystalname.xtl, ./tmp???, ???.lab.

SEE ALSO

sort(1).

ENVIRONMENT

LAUEVIEWHOME

To get man page from $LAUEVIEWHOME/man and get symmlib from $LAUEVIEWHOME/lib require the environment value set correctly.

CRYSTALNAME

If -i option is used but no crystal name is followed, the program will try to load xtal_info file $CRYSTALNAME.xtl.

CRYSTALINFO

With -i option on, the program will try to load xtal_info file from the current directory. If not found, it will try again from the directory $CRYSTALINFO.

BUGS

Numerical data only. Any character string in the data file(s) will cause read error, but this will not abort the program. The records with character strings are ignored. And also they are kept in the output file(s).

The maximum record length of the input data file is 300 characters. The extra part of any longer record will be ignored.