Chapter 3.7

LAZY-PULVERIX

A program to calculate theoretical X-ray and neutron diffraction powder patterns

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For a further description of the program see *J.Appl.Cryst.* (**1977**), *10*, 73-74

LAZY-PULVERIX consists of two programs

- **LAZY** - decodes the input data and prepares the data file for **PULVERIX**.
- **PULVERIX** - reads the file from **LAZY** and calculates the powder pattern.

3.6.1 Instructions Summary

3.6.1.1 General remarks

Calculations for several structures may be done in one run, the order in which the data instructions are given within a set is not important. When reading the data instructions, the program identifies the kind of data instruction by labels in columns 1-6 (e.g. TITLE, CONDIT, CELL, SPCGRP etc.). One END instruction must terminate each set and one FINISH instruction must follow the last END instruction.

The format of the TITLE, CELL, LATICE, SYMTRY, SPCGRP, ATOM, END and FINISH instructions are compatible with the corresponding format of the X-RAY 76 program system, except small differences in certain prescriptions (see CELL and ATOM instructions). The minimum of input must contain TITLE, CELL, SPCGRP, ATOM, END and FINISH instructions. The SPCGRP instruction may be replaced by LATICE and SYMTRY instructions and vice versa.

TITLE instruction - title

```
format(a2,a3,1x,17a4)
   cols
   1- 5  title     punch instruction label TITLE
   7-74  compnd    any alphanumeric information  (for instance the
                   name of the substance)
```

CONDIT instruction - experimental conditions

```
format(3a2,4x,a4,f6.0,2f5.0,1x,a1,i2,a2,1x,a1)
    cols
   1- 6  condit    punch instruction label  CONDIT
  11-14  symwl     symbol for wavelength
                            adjust to the left of the field.
                            example
                            CUA1 = Copper Kα1 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 Cukα X-radiation is assumed.

                          neutron diffraction
                          leave columns 11-14 blank and give
                          value of wavelength in columns 15-20.
  15-20  wl        wavelength in Angstrom
                          need not be given if symwl is specified
  21-25  tl        lower theta -limit of calculation
  26-30  th        upper theta -limit of calculation
                          if left blank  tl=0 and th=89 degrees.
                          for Guinier cameras th is 45 degrees
     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
  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
  35-36  symlp     experimental techniques
                         blank    Debye-Scherrer or powder-diffractometer
                          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
     38  iano      correction for anomalous dispersion (x rays only)
                          blank   correction is made
                          N       no correction is made.
```

Notes

- It is recommended to compute all structures with neutral atoms. If form-factors for ionized atoms are used, the program will not make dispersion corrections. No dispersion correction will be made for neutron diffraction.
- If no CONDIT instruction is given, Cu-Kα radiation and Debye-Scherrer technique is assumed. A correction for anomalous dispersion will be made and a complete powder pattern will be calculated.

CELL instruction - lattice constants

```
format(3a2,7x,3f8.0,3f9.0)
   cols
   1- 4  cell      punch instruction label CELL
  14-21  a         lattice parameters in Angstrom and degrees
  22-29  b                  cubic        omit b,c,alpha,beta,gamma
  30-37  c                  hexagonal    omit b,alpha,beta,
                                              and set gamma=120.
                            rhombohedral see note below
  38-46  alpha              tetragonal   omit b,alpha,beta,gamma
  47-55  beta               orthorhombic omit alpha,beta,gamma
  56-64  gamma              monoclinic   omit alpha,gamma
```

- Rhombohedral should be calculated with hexagonal axes. If rhombohedral axes are desired the structure must be described in the triclinic system.

LATICE instruction - symmetry center and Bravais lattice (this instruction may be replaced by a SPCGRP instruction)

```
format(3a2,2x,a1,2x,a1)
   cols
   1- 6  latice    punch instruction label  LATICE
      9  isymce    center of symmetry at origin
                             C   yes (centric)
                             A   no (acentric)

     12  symbr     bravais lattice indicator
                             P   primitive
                             I   body centered
                             R   rhombohedral
                             F   face centered
                             A   a centered
                             B   b centered
                             C   c centered
                             blank   primitive
```

For trigonal case

- P space groups give hexagonal lattice constants and set symbr=P
- R space groups :
    1. hexagonal cell set symbr=R. The program assumes the standard (obverse) setting.
    2. rhombohedral cell set symbr=P and give a,b, c and angles explicitly on CELL instruction (triclinic description).

If no LATICE instruction is given, a non centrosymmetric structure and a primitive lattice is assumed.

SYMTRY instruction - equivalent point positions (these instructions may be replaced by a SPCGRP instruction)

```
format(3a2,45a1)
   cols
   1- 6  symtry    punch instruction label  SYMTRY
   7-51  ipos      equivalent position coded in verbatim form.
                             include one instruction for each position.

                             rules for coding
                             coordinates are separated by commas,
                             fractions are written as two integers
                                       separated by a slash.
                             blank spaces are ignored.

                             example     space group p 21/c
                                 SYMTRY  X, Y, Z
                                 SYMTRY  X,1/2-Y,1/2+Z
```

- If isymce=C then only one of any two centrosymmetric positions need to be given. If symbr= I,R,F,A,B or C, only one of the positions related by centering needs to be given
- If no SYMTRY instruction is given, x,y,z is automatically assumed, however if SYMTRY instructions are given then the x,y,z position MUST be included.

SPCGRP instruction - space group (this instruction may replace LATICE and SYMTRY instructions)

```
format(3a2,35a1)
   cols
   1- 6  spcgrp    punch instruction label SPCGRP
   8-17  ipos      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

                             the list of allowed symbols is given at
                             the end of this description.
```

- For all other symbols the program may generate wrong equipoints without error messages.
- For non standard space group settings SYMTRY and LATICE instructions MUST be used.
- For centrosymmetric groups, the program assumes the setting having 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 instructions corresponding to a triclinic description.

ATOM instruction - atom identifier and coordinates (use one atom instruction for each atom in the asymmetric unit).

```
format(3a2,1x,a4,a2,3f8.0,f6.0,f5.0)
   cols
   1- 4  atom      punch instruction label  ATOM
   8-11  elemt     symbol of element and ionisation state
                             adjust to the left of the field.
                             examples
                                 CA   symbol for calcium(neutral)
                                 CA2+ symbol for calcium(ionized)
                             only symbols listed in the table for
```

```
                                atom identification at the end of
                                this description can be given.
 12-13  ide      sequence number or atom label. (may be left blank)
                           it is convenient to number or label
                           atoms of the same type.

 14-21  x        x coordinate
 22-29  y        y coordinate
 30-37  z        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
 38-43  btemp    Webye-Waller factor
                  If left blank  no temperature factor correction
                  will be made.
 44-48  foccu    occupation factor
                  This factor is usually 1 (=full occupancy of the
                  site) but it may be smaller in disordered struc-
                  tures. If left blank full occupancy will be assumed
```

END instruction - terminates each set of data instructions

```
  cols
 1- 3  end       punch instruction label  END
```

FINISH instruction - terminates the run

```
cols
   1- 6  finish    punch instruction label FINISH
```

Note
This instruction must come after the last end instruction. It initiates execution of the program.

3.6.2 List of allowed symbols

3.6.2.1 Wavelengths (variable symwl on CONDIT instruction)

The lines contain the symbols for Kα1, Kα2 and the weighted average of the Kα 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)
```

3.6.2.2. ATOM identification (variable elemt on ATOM instruction)

The atom symbols are used to retrieve the scattering factors for X-rays and the nuclear (but not the magnetic) scattering factors for neutrons. Do NOT include the asterisk preceeding 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.

```
*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+
```

Symbols with special meaning

```
H.    Hydrogen HF scattering factor
C.    Carbon   HF scattering factor
SI.   Silicon  HF scattering factor
D.    Deuterium (for neutron diffraction ONLY)
O2-.  taken from Acta Cryst. vol.19, p.486(1965).
```

3.6.2.3 SPACE GROUP symbols (variable ipos on SPCGRP instruction)

Do NOT include the star preceeding some of the symbols. The star indicates centro-symmetric space groups which have been described with several settings. The program generates only the setting with the centre of symmetry at the origin of the unit cell. WARNING - a symbol that does not figure in this list may yield wrong equipoints.

```
   TRICLINIC
    P 1          P -1

  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  POINT  POSITIONS  GENERATED  FROM  THESE  SYMBOLS  CORRESPOND  TO  THE
MONOCLINIC SETTING WITH B AS UNIQUE AXIS (ALPHA=GAMMA=90.)

   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

    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

  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
 ALL R-SPACE GROUPS REFER TO THE HEXAGONAL SETTING
    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

    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
```

3.6.3 Formulae for the Lorentz-polarisation factors

3.6.3.1 Debye-Scherrer technique

$l = 1.0/(\sin^2\theta \times \cos\theta)$
$p = (1.0+ \cos^2 2\theta)/2.$

3.6.3.2 Guinier technique

$l = 1./(\sin^2\theta \times \cos\theta \times \cos(2\theta-\beta))$

β = angle between the normal to the specimen and the direction of the incident beam.

$p = (1.0+ \cos^2 2\theta \times \cos^2 2\alpha)/(1+\cos^2 2\alpha)$

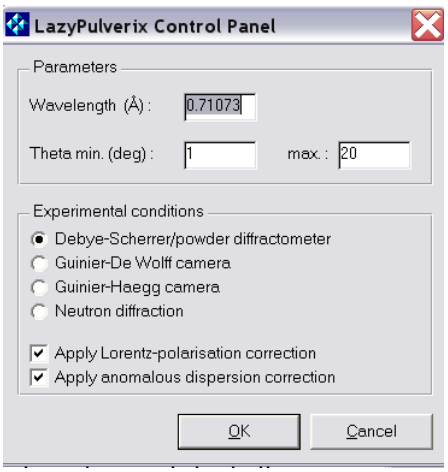
α = diffraction angle of monochromator.

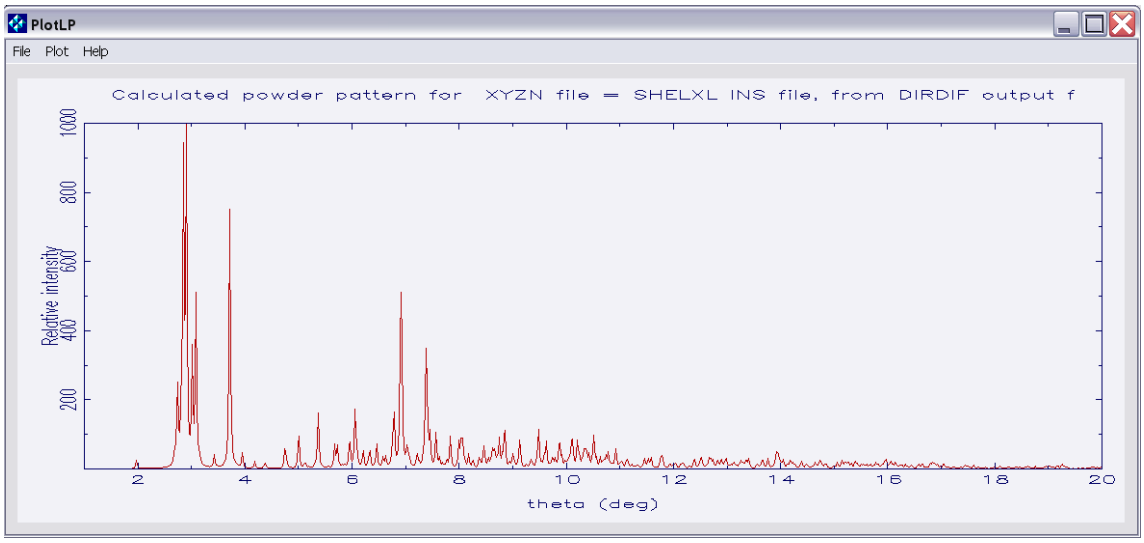
α and β depend on the geometry of the Guinier camera and the d spacing of the reflecting planes of the monochromator crystal. For Guinier cameras other than Guinier-de Wolff or Guinier-Haegg or for monochromator crystals other than quartz changes in the program have to be made (see *remarks for adapting the program* in the source deck of PULVERIX).

3.6.4. LAZY-PULVERIX implementation in WinGX

The programs **LAZY** and **PULVERIX** have been compiled essentially unaltered, but the limits have been substantially increased. A maximum of 5000 reflections may be calculated, up to 1000 atoms of one type may be entered, and 20 different atomic types are allowed. A new program **PLOTLP** has been written which plots the calculated intensities listed in the output file of **PULVERIX** (called *PULVERIX.LST*). This program is run automatically after **LAZY** and **PULVERIX**. Lineshapes may be Lorentzian, Gaussian or a 50:50 mix and linewidths may be varied. Monochrome or colour PostScript files may also be written. The plot parameters may be selected from the Plot[Parameters] sub-menu.

The program instructions are written by the GUI shown below, and the above input description is for informational purposes only. The calculated spectrum is displayed as a plot, which may be saved in PostScript format.





3.6.5. Disclaimer

Although the program 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 equi-points used by the program are part of the output (file *PULVERIX.LST*) and the user is advised to compare them with the values given in the International Tables for Crystallography.