PSM3

I. Description

The aim of this program is the electron diffraction data, to calculate the scale factors between electron diffraction patterns obtained after rotation around a specific axe of the reciprocal, to merge the data according to symmetry.

This program uses the data from EXTRAX, an ImageJ plugin available at:
http://rsbweb.nih.gov/ij/download.html
http://rsb.info.nih.gov/ij/plugins/extrax/index.html

The files ("out" extension) contain at least 9 columns « h k l I Poisson(I) bg Sigma(bg) g d (X Y) ».

Ex :

```
;
;h  k   l   I       Poisson(I)  bg      Sigma(bg)   g(?-1)       d(?)
;
-13 0   -3  7600        112     4947        47480       1.89883732  0.52663806
-13 0   -2  -1923       82      8625        45258       1.87287365  0.53393885
-13 0   -1  5470        111     6762        45073       1.86010184  0.53760497
-12 0   -4  2831        100     7206        44694       1.80419248  0.55426459
-12 0   -3  4367        89      3482        47000       1.76846659  0.56546163
```

II. How to use it

- Put PSM3.exe in the the same directory as the file to be treated then double click on it.
- Put PSM3.exe in a directory situated in the PATH. The program can then run with the command line from every location. There is no need to copy paste PSM3.exe in many directory.
    - From command line, move to your work directory and type PSM3.
    - You can also right click on the input file "2d.txt" with the mouse → open with → select a program → browse → go to PSM3.exe.

To put a directory in the PATH :
Right Click on the workstation → Properties → Avanced → left click on environment variables → click on path and modify then type ";" then the directory path and save.
Or in "Start" "Search" type "cmd" then, in the open window, type :

PATH=%PATH%;directory_path

III. Input File

PSM3 need an input file that contains the name of the files to be treated (with the extension). This input files has to be located in the the same directory as the files.

Example : 2d.txt

zap1-2d.out
zap2-2d.out
zap3-2d.out
zap4-2d.out
zap5-2d.out
zap6-2d.out
zap7-2d.out

IV. Data Treatments

Each file can undergo many treatments before the calculation of scale factors. There is "g" limits (g=1/d), suppression of negative reflections and geometric correction can be applied. Scale factors can be calculated from the whole data or only from the most intense reflections. The Friedel pair can also be merged (distances and intensities). Forbidden reflections are suppressed according to the space group. The suppressed reflections are displayed in the command line window.

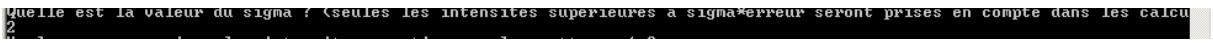
1) g limits

Only reflections with a g value in the range g_{min}-g_{max} are kept for calculations. The others are deleted.

Here the limits are 0 and 8$Å^{-1}$.

2) Reflections intensities restrictions

Enter a *sigma* value. Reflections that have intensity below *sigma×error* are not taken into account in the scale factor calculation, but the are not deleted.

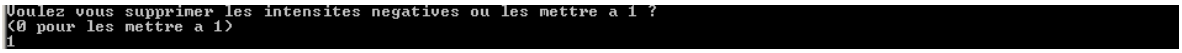


Here, reflections that have intensity below two times the error are not taken into account.

3) Negative intensities reflections suppression

If the the data set contains negative reflections, you have two choices:

- delete these reflections.
- or keep them and give them a week intensity. In PSM3, this week intensity is 1.



Here, negative reflections are deleted.

4) Geomerical corrections

It is possible to apply geometrical corrections linked to the precession geometry. The Gjonnes approximation can be applied to each file.

$$C = g\sqrt{1-\left(\frac{g}{2\times R_{Ewald}\times\varphi}\right)^2} \qquad \text{Gjonnes approximation}$$

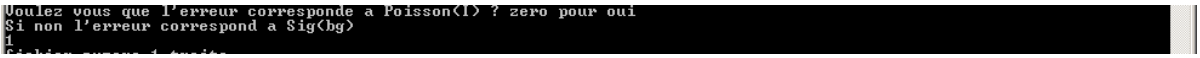
$$I_{cor} = C\times I_{\exp}$$

Where R_{Ewald} is the radius of the Ewald sphere and φ is the semi-angle precession.

Here, we do not apply corrections.

5) Choice of the error

You can choice the reflection intensity error between the Poisson value (square root of the intensity) and the standard deviation of the background calculated in EXTRAX.



Here, the error is the standard deviation of the background.

6) Merge of the Friedel pairs

Although the precession reduce misorientation effects on diffraction patterns, they still exist. PSM3 allow to merge intensities of the Friedel pairs to reduce misorientaion effects. Moreover, the g distances are no longer calculated from the valur given by EXTRAX but from XY position of each Friedel pairs.

7) Choice of the Space Group

You can choose a space group from its number to delete the forbidden reflections and merge equivalent reflection.

Non-standard space groups like $P2_1/n$ ($P2_1/c$) or Pbnm (Pnma) can not be chosen.

```
Quel est le numero du groupe d'espace ?
100
```

Here, the space group is P4bm.

A space group list is provided at the end of this document.

The program treats the data and a sentence is displayed when the treatment is done. An hkl file is created for each input (zap1-2d.out.hkl). Finally, the output file name is asked.

```
cond vaut : 4
  -5    0   -5        295.00         33.00        811.00        973.00     1.34235399     0.74495998    122.00    821.00
  -3    0   -3       -337.00         52.00       3059.00       1515.00     0.80835032     1.23708741    296.00    709.00
  -1    0   -1      32977.00        209.00      10613.00      14148.00     0.27223501     3.67329687    470.00    598.00
   1    0    1      15731.00        146.00       5553.00       7690.00     0.27292294     3.66403792    644.00    487.00
   3    0    3        491.00         56.00       2677.00       1311.00     0.80821625     1.23729261    818.00    375.00
   5    0    5        -73.00         29.00        935.00       1023.00     1.33512312     0.74899460    993.00    264.00
cond vaut : 10
   0   -5    5        361.00         34.00        820.00        927.00     1.30970127     0.76353289    837.00    108.00
   0   -3    3        314.00         57.00       2929.00       1445.00     0.76806733     1.30196919    725.00    281.00
   0   -1    1      -8029.00        132.00      25422.00      16134.00     0.24623325     4.06119001    613.00    455.00
   0    1   -1      -7273.00        132.00      24794.00      15324.00     0.29847093     3.35040998    502.00    629.00
   0    3   -3        765.00         58.00       2645.00       1340.00     0.83655549     1.19537797    390.00    803.00
   0    5   -5        133.00         31.00        837.00        907.00     1.37371606     0.72795247    278.00    977.00
cond vaut : 0
fichier numero 6 traite

Quel est le nom du fichier de sortie ? (PSMsortie par defaut)
```

Forbidden reflections are displayed.

V. Output files

PSM3 creates automatically many output files in addition to the previous citated:

Output_name.hkl, file containing the whole scaled reflections.

Output_name.txt, file containing the treatments parameters and the results of the scale factor calculations.

*Output_name*fin.hkl, file containing the reducted data.

and *Output_name*-g.txt, file containing the result of scale factor calculations on the g values. (These calculations are made in order to take into account the slight variations of the microscope constant from a pattern to the next).

VI. Scale factors calculation

The scale factors are calculated by linear least square method. The following formula is minimized:

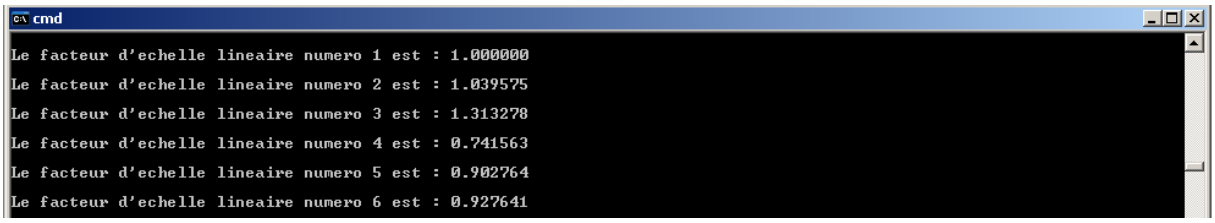
$$S = \sum_n \sum_m \left(A_m \alpha_{nm} - A_n \right)^2$$

A_m is the scale factor of the pattern number m.

α_{nm} is the weight mean (Intensity/error) of intensities ratio between common reflections of patterns number n and m.

VII. Réduction des données en fonction de la symétrie

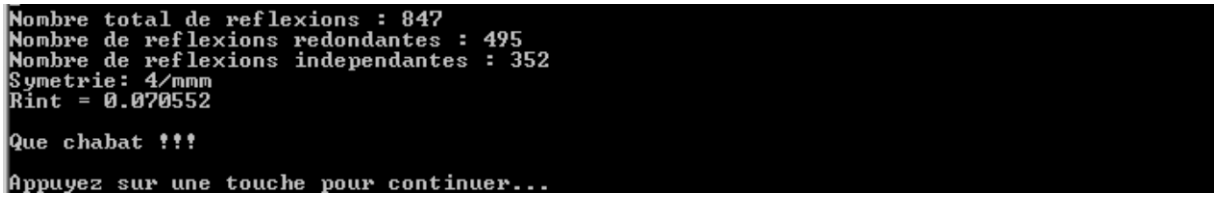
Equivalent reflections intensities are merged to the mean value.



finally, the total number of reflections, the number of redundant reflections, the number of independent reflections, the symmetry and the Rint are displayed.

$$R\,\mathrm{int} = \frac{\sum_{ind}\left(\frac{1}{n}\sum_{eq}\left|I - < I >\right|\right)}{\sum_{ind}\left(\frac{1}{n}\sum_{eq} I\right)}$$

ind are the independent reflections, *eq* are the equivalent reflections, *n* is the number of equivalent reflections and I is the diffracted intensity of the considered reflection.



"Que chabat" means that "It's finish".

SPACE GROUP LIST :

Triclinic and monoclinic :

1: P1 2: P-1 3: P2 4: P21 5: C2 6: Pm 7: Pc 8: Cm 9: Cc 10: P2/m 11: $P2_1/m$ 12: C2/m 13: P2/c 14: $P2_1/c$ 15: C2/c

Orthorhombic :

16: P222 17: $P222_1$ 18: $P2_12_12$ 19: $P2_12_12_1$ 20: $C222_1$ 21: C222 22: F222 23: I222 24: $I2_12_12_1$ 25: Pmm2 26: $Pmc2_1$ 27: Pcc2 28: Pma2 29: $Pca2_1$30: Pnc2 31: $Pmn2_1$ 32: Pba2 33: $Pna2_1$ 34: Pnn2 35: Cmm2 36: $Cmc2_1$ 37: Ccc2 38: Amm2 39: Aem2 40: Ama2 41: Aea2 42: Fmm2 43: Fdd2 44: Imm2 45: Iba2 46: Ima2 47: Pmmm 48: Pnnn 49: Pccm 50: Pban 51: Pmma 52: Pnna 53: Pmna 54: Pcca 55: Pbam 56: Pccn 57: Pbcm 58: Pnnm 59: Pmmn 60: Pbcn 61: Pbca 62: Pnma 63: Cmcm 64: Cmce 65: Cmmm 66: Cccm 67: Cmme 68: Ccce 69: Fmmm 70: Fddd 71: Immm 72: Ibam 73: Ibca 74: Imma

Teragonal :

75: P4 76: P41 77: P42 78: P43 79: I4 80: I41 81: P-4 82: I-4 83: P4/m 84: $P4_2/m$ 85: P4/n 86: $P4_2/n$ 87: I4/m 88: $I4_1/a$ 89: P422 90: $P4_212$ 91: $P4_122$ 92: $P4_12_12$ 93: $P4_222$ 94: $P4_22_12$ 95: $P4_322$ 96: $P4_32_12$ 97: I422 98: $I4_122$ 99: P4mm 100:P4bm 101: $P4_2cm$ 102: $P4_2nm$ 103: P4cc 104: P4nc 105: $P4_2mc$ 106: $P4_2bc$ 107: I4mm 108: I4cm 109: $I4_1md$ 110: $I4_1cd$ 111: P-42m 112: P-42c 113: $P-42_1m$ 114: $P-42_1c$ 115: P-4m2 116: P-4c2 117: P-4b2 118: P-4n2 119: I-4m2 120: I-4c2 121: I-42m 122: I-42d 123: P4/mmm 124: P4/mcc 125: P4/nbm 126: P4/nnc 127: P4/mbm 128: P4/mnc 129: P4/nmm 130: P4/ncc 131: $P4_2/mmc$ 132: $P4_2/mcm$ 133: $P4_2/nbc$ 134: $P4_2/nnm$ 135: $P4_2/mbc$ 136: $P4_2/mnm$ 137: $P4_2/nmc$ 138: $P4_2/ncm$ 139: I4/mmm 140: I4/mcm 141: $I4_1/amd$ 142: $I4_1/acd$

Rhomboedral :

143: P3 144: P31 145: P32 146: R3 147: P-3 148: R-3 149: P312 150: P321 151: $P3_112$ 152: $P3_121$ 153: $P3_212$ 154: $P3_221$ 155: R32 156: P3m1 157: P31m 158: P3c1 159: P31c 160: R3m 161: R3c 162: P-31m 163: P-31c 164: P-3m1 165: P-3c1 166: R-3m 167: R-3c

Héxagonal :

168: P6 169: $P6_1$ 170: $P6_5$ 171: $P6_2$ 172: $P6_4$ 173: $P6_3$ 174: P-6 175: P6/m 176: $P6_3/m$ 177: P622 178: $P6_122$ 179: $P6_522$ 180: $P6_222$ 181: $P6_422$ 182: $P6_322$ 183: P6mm 184: P6cc 185: $P6_3cm$ 186: $P6_3mc$ 187: P-6m2 188: P-6c2 189: P-62m 190: P-62c 191: P6/mmm 192: P6/mcc 193: $P6_3/mcm$ 194: $P6_3/mmc$

Cubic :

195: P23 196: F23 197: I23 198: $P2_13$ 199: $I2_13$ 200: Pm-3 201: Pn-3 202: Fm-3 203: Fd-3 204: Im-3 205: Pa-3 206: Ia-3 207: P432 208: $P4_232$ 209: F432 210: $F4_132$ 211: I432 212: $P4_332$ 213: $P4_132$ 214: $I4_132$ 215: P-43m 216: F-43m 217: I-43m 218: P-43n 219: F-43c 220: I-43d 221: Pm-3m 222: Pn-3n 223: Pm-3n 224: Pn-3m 225: Fm-3m 226: Fm-3c 227: Fd-3m 228: Fd-3c 229: Im-3m 230: Ia-3d