◎プログラム PFLS（試料２）の実行例

```
Microsoft Windows XP [Version 5.1.2600]
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c:¥xbin>pflsxe  ←コマンドプロンプト画面にて pflsx と入力して、プログラム pflsx.exe
を実行します

**********************************************************************
*                                                                    *
*                  Computer Program PFLS (ver.5.00)                  *
*                                                                    *
*                       for Rietveld Refinement                      *
*                                                                    *
*                           By H.Toraya                              *
*                                                                    *
**********************************************************************

  Input job title (memorandum) in 70 characters.
            ←ジョブタイトルを入力します（省略可)。


  Input the filename of the intensity data.
110608.dat  ←解析するＸ線回折データのファイル名を入力します。

  Intensity data were read.   N =  5001

  File name of profile intensity data: 110608.dat
  NTB-1+corundum=8:2

  2theta-s  2theta-e    Step    Time  Nobs     Lambda1    Lambda2   I2/I1
    15.000   115.000   0.020     2.0  5001    1.540562   1.544390   0.497
```

Ti (+4e)

18.000	17.808	17.255	16.403	15.342	14.170	12.979	11.844
10.815	9.917	9.158	8.529	8.012	7.588	7.234	6.930
6.664	6.419	6.189	5.965	5.745	5.525	5.306	5.087
4.870	4.655	4.443	4.236	4.035	3.841	3.655	3.478

O (-2e)

10.000	9.633	8.671	7.423	6.174	5.081	4.192	3.498
2.968	2.569	2.274	2.053	1.891	1.768	1.676	1.603
1.543	1.492	1.447	1.406	1.367	1.329	1.291	1.253
1.216	1.179	1.142	1.105	1.068	1.031	0.995	0.959

Al (+3e)

10.000	9.933	9.738	9.424	9.011	8.520	7.975	7.399
6.813	6.237	5.683	5.162	4.681	4.243	3.851	3.503
3.195	2.926	2.693	2.492	2.319	2.169	2.041	1.931
1.837	1.755	1.685	1.624	1.570	1.522	1.479	1.438

Df" :	0.189	0.047	0.204
Df"":	1.807	0.032	0.246

Space group: Pbca (No. 61) Centro symmetric

Symmetry Operations:

No.	R11	R12	R13	R21	R22	R23	R31	R32	R33	T1	T2	T3
1	1	0	0	0	1	0	0	0	1	0.0000000	0.0000000	0.0000000
2	1	0	0	0	-1	0	0	0	-1	0.5000000	0.5000000	0.0000000
3	-1	0	0	0	1	0	0	0	-1	0.0000000	0.5000000	0.5000000
4	-1	0	0	0	-1	0	0	0	1	0.5000000	0.0000000	0.5000000

Space group: I41/amd (No.141) Centro symmetric

Symmetry Operations:

No.	R11	R12	R13	R21	R22	R23	R31	R32	R33	T1	T2	T3
1	1	0	0	0	1	0	0	0	1	0.0000000	0.0000000	0.0000000
2	-1	0	0	0	-1	0	0	0	1	0.0000000	0.0000000	0.0000000
3	1	0	0	0	1	0	0	0	-1	0.0000000	0.5000000	0.2500000
4	-1	0	0	0	-1	0	0	0	-1	0.0000000	0.5000000	0.2500000
5	-1	0	0	0	1	0	0	0	1	0.0000000	0.0000000	0.0000000
6	1	0	0	0	-1	0	0	0	1	0.0000000	0.0000000	0.0000000
7	-1	0	0	0	1	0	0	0	-1	0.0000000	0.5000000	0.2500000
8	1	0	0	0	-1	0	0	0	-1	0.0000000	0.5000000	0.2500000
9	0	1	0	1	0	0	0	0	-1	0.0000000	0.0000000	0.0000000
10	0	-1	0	-1	0	0	0	0	-1	0.0000000	0.0000000	0.0000000
11	0	1	0	1	0	0	0	0	1	0.0000000	0.5000000	0.2500000
12	0	-1	0	-1	0	0	0	0	1	0.0000000	0.5000000	0.2500000
13	0	-1	0	1	0	0	0	0	-1	0.0000000	0.0000000	0.0000000
14	0	1	0	-1	0	0	0	0	-1	0.0000000	0.0000000	0.0000000
15	0	-1	0	1	0	0	0	0	1	0.0000000	0.5000000	0.2500000
16	0	1	0	-1	0	0	0	0	1	0.0000000	0.5000000	0.2500000
17	1	0	0	0	1	0	0	0	1	0.5000000	0.5000000	0.5000000
18	-1	0	0	0	-1	0	0	0	1	0.5000000	0.5000000	0.5000000
19	1	0	0	0	1	0	0	0	-1	0.5000000	0.0000000	0.7500000
20	-1	0	0	0	-1	0	0	0	-1	0.5000000	0.0000000	0.7500000
21	-1	0	0	0	1	0	0	0	1	0.5000000	0.5000000	0.5000000
22	1	0	0	0	-1	0	0	0	1	0.5000000	0.5000000	0.5000000
23	-1	0	0	0	1	0	0	0	-1	0.5000000	0.0000000	0.7500000
24	1	0	0	0	-1	0	0	0	-1	0.5000000	0.0000000	0.7500000
25	0	1	0	1	0	0	0	0	-1	0.5000000	0.5000000	0.5000000
26	0	-1	0	-1	0	0	0	0	-1	0.5000000	0.5000000	0.5000000
27	0	1	0	1	0	0	0	0	1	0.5000000	0.0000000	0.7500000
28	0	-1	0	-1	0	0	0	0	1	0.5000000	0.0000000	0.7500000
29	0	-1	0	1	0	0	0	0	-1	0.5000000	0.5000000	0.5000000
30	0	1	0	-1	0	0	0	0	-1	0.5000000	0.5000000	0.5000000

31	0	-1	0	1	0	0	0	0	1	0.5000000	0.0000000	0.7500000
32	0	1	0	-1	0	0	0	0	1	0.5000000	0.0000000	0.7500000

Space group: R-3c (No.167) Centro symmetric

Symmetry Operations:

No.	R11	R12	R13	R21	R22	R23	R31	R32	R33	T1	T2	T3
1	1	0	0	0	1	0	0	0	1	0.0000000	0.0000000	0.0000000
2	0	-1	0	1	-1	0	0	0	1	0.0000000	0.0000000	0.0000000
3	-1	1	0	-1	0	0	0	0	1	0.0000000	0.0000000	0.0000000
4	0	-1	0	-1	0	0	0	0	1	0.0000000	0.0000000	0.5000000
5	1	0	0	1	-1	0	0	0	1	0.0000000	0.0000000	0.5000000
6	-1	1	0	0	1	0	0	0	1	0.0000000	0.0000000	0.5000000
7	1	0	0	0	1	0	0	0	1	0.3333333	0.6666667	0.6666667
8	0	-1	0	1	-1	0	0	0	1	0.3333333	0.6666667	0.6666667
9	-1	1	0	-1	0	0	0	0	1	0.3333333	0.6666667	0.6666667
10	0	-1	0	-1	0	0	0	0	1	0.3333333	0.6666667	0.1666667
11	1	0	0	1	-1	0	0	0	1	0.3333333	0.6666667	0.1666667
12	-1	1	0	0	1	0	0	0	1	0.3333333	0.6666667	0.1666667
13	1	0	0	0	1	0	0	0	1	0.6666667	0.3333333	0.3333333
14	0	-1	0	1	-1	0	0	0	1	0.6666667	0.3333333	0.3333333
15	-1	1	0	-1	0	0	0	0	1	0.6666667	0.3333333	0.3333333
16	0	-1	0	-1	0	0	0	0	1	0.6666667	0.3333333	0.8333334
17	1	0	0	1	-1	0	0	0	1	0.6666667	0.3333333	0.8333334
18	-1	1	0	0	1	0	0	0	1	0.6666667	0.3333333	0.8333334

---------- Input profile and strutural parameters ----------

Select a file name for profile parameters
0:file A, 1:file B, 2:file C, 3:your option.
1

Profile parameters were read from a file: reflexb.d

```
  Select a filename for strutural parameters:
    0:file A,   1:file B,   2:file C,   3:your option.
1

  Atomic parameters were read from datafile: atomsb.d


--------------- Set 2-theta range for analysis ------------------------

  The 2theta-range of intensity  data =  15.000 to 115.000
  The 2theta-range of reflection data =  10.000 to 130.000

  Input low- and high-angle limits of the 2theta range,
    which is to be used for whole-powder-pattern fitting.
15
110  ←解析２θ範囲を指定します。ここでは、例えば、２θ＝１５～１１０°と入力して
います

  2theta-L  2theta-H    Nobs        Y(max) at 2theta    Y(min) at 2theta
    15.000   110.000    4751        11271.    25.520      112.    89.980


--------------- Correction of parameters before the l.s. ---------------

   -1: terminate job (results will be aborted)
    0: no change
    1: correct global and profile parameters
    2: correct structural parameters
    3: correct scale, OATM, or texture parameters
    4: see the pattern before the l.s.
    5: how to change parameter values ?
0


--------------- Set calculation conditions ----------------------------
```

```
  Calculation of profile function is truncated
  when profile intensity < Y(lim) (unit = counts).

  Damping factors (DF) will be applied when parameters
  oscillate or are apt to diverge during the least-squares.

  Y(lim)  D.F.  bj    tj  I2I1  Cell  FWHM  Ae/m axyzB  Scal  OATM  Xtex
     1.5      1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00


  Enter number to change parameters:
    0: no change,   1: Y(lim),   2: D.F.
2

  Input D.F. (default = 1.0) for
    bj, tj, E, cell, FWHM, Ae/m, axyzB, Scale, OATM, Xtex.
0 0 0 0 0.5 0.5 0 0 0 0  ←ピークプロファイルの形状パラメータである半値幅(FWHM)と
非対称性(Ae/m)について、ダンピングファクターを 0.5 に設定した例です。

  Y(lim)  D.F.  bj    tj  I2I1  Cell  FWHM  Ae/m axyzB  Scal  OATM  Xtex
     1.5      1.00  1.00  1.00  1.00  0.50  0.50  1.00  1.00  1.00  1.00


  Enter number to change parameters:
    0: no change,   1: Y(lim),   2: D.F.
0

--------------- Optimization was started -----------------------------

  Select a mode of refinement:
    -3: terminate/pause l.s. cycles
    -2: full-manual (single-step)
    -1: manual
     0: automatic
0
```

```
 Lp correction (normal):  A part =   1.000  B part =   0.790

! 184 reflections were omitted because of |F| = 0.

-----------------------------------------------------------------------
 Parameter selection in cycle  1:  nr = 15
 gp   1   2   3   4   5   6   0   0   0   0   0
 pp   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0
 tp   7   0
 sp   0   0   0   0   0       0   0   0   0   0       0   0   0   0   0

 pp   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0
 tp   8   0
 sp   0   0   0   0   0       0   0   0   0   0
 pp   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0
 tp   9   0
 sp   0   0   0   0   0       0   0   0   0   0

 L.S.       Ncyl Nobs Npar Nvar       Rp     Rwp     Rp"      Re      GOF
 Before cyl    1 4751 4229    9  0.87332 0.88323 0.93711 0.03769  23.437

           Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
              1  166           1.00000 0.10641 0.89358 0.89435 0.69801

           Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
              2   27           1.00000 0.17371 0.82629 0.82629 0.58755

           Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
              3   44           1.00000 0.19283 0.80717 0.80717 0.58676

 Change of l.s. parameters in cycle  1
  Com.  Atoms  Para         old      change         new      e.s.d.

                 b0    0.000000    3.170267    3.170267    0.138118 >5%
                 b1    0.000000   -3.463466   -3.463466    0.486313 >5%
                 b2    0.000000    0.855841    0.855841    0.794871 >5%
```

	b3	0.000000	0.945484	0.945484	1.906739	>5%
	b4	0.000000	-0.949821	-0.949821	0.856910	>5%
	b5	0.000000	1.105556	1.105556	1.661390	>5%
1	Scale	1.000000	3.234054	4.234055	0.197435	>5%
2	Scale	1.000000	0.798181	1.798181	0.127806	>5%
3	Scale	1.000000	1.263214	2.263214	0.154267	>5%

Lp correction (normal): A part = 1.000 B part = 0.790

Parameter selection in cycle 2: nr = 14

gp	1	2	3	4	5	6	7	0	0	0	0						
pp	8	9	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0
tp	11	0															
sp	0	0	0	0	0		0	0	0	0	0		0	0	0	0	0
pp	12	12	13	0	0	0	0	0	0	0	0	0	0	0	0	0	0
tp	14	0															
sp	0	0	0	0	0		0	0	0	0	0						
pp	15	15	16	0	0	0	0	0	0	0	0	0	0	0	0	0	0
tp	17	0															
sp	0	0	0	0	0		0	0	0	0	0						

L.S.	Ncyl	Nobs	Npar	Nvar	Rp	Rwp	Rp"	Re	GOF
Before cyl	2	4751	4467	17	0.28765	0.34367	0.60029	0.03765	9.127

Comp	Nref	SumIo	: SumIc	SumdI	RBragg	RF
1	147	1.00000	0.73695	0.26305	0.36153	0.19418

Comp	Nref	SumIo	: SumIc	SumdI	RBragg	RF
2	26	1.00000	0.72747	0.27253	0.31664	0.14859

Comp	Nref	SumIo	: SumIc	SumdI	RBragg	RF
3	35	1.00000	0.91223	0.08777	0.18458	0.12291

Change of l.s. parameters in cycle 2

Com.	Atoms	Para	old	change	new	e.s.d.	
		b0	3.170267	-0.063879	3.106388	0.054019	>5%
		b1	-3.463466	0.085113	-3.378353	0.189588	>5%
		b2	0.855841	0.037022	0.892862	0.309633	>5%
		b3	0.945484	-0.179576	0.765908	0.742926	>5%
		b4	-0.949821	0.018398	-0.931423	0.333794	>5%
		b5	1.105556	0.097975	1.203531	0.647242	>5%
		t0	0.000000	-0.008390	-0.008390	0.004071	>5%
1		a	9.174000	-0.007384	9.166616	0.002203	>5%
1		b	5.449000	-0.008154	5.440846	0.001218	>5%
1		c	5.138000	0.007334	5.145334	0.001002	>5%
1		Scale	4.234055	0.079588	4.313642	0.078186	>5%
2		a	3.785000	0.004771	3.789772	0.000681	>5%
2		b	3.785000	0.004771	3.789772	0.000000	
2		c	9.515000	-0.009481	9.505519	0.002419	>5%
2		Scale	1.798181	0.040697	1.838878	0.051225	>5%
3		a	4.759000	0.000534	4.759533	0.000359	>5%
3		b	4.759000	0.000534	4.759533	0.000000	
3		c	12.991000	0.001632	12.992633	0.001373	>5%
3		Scale	2.263214	0.100039	2.363253	0.060736	>5%

Lp correction (normal): A part = 1.000 B part = 0.790

Parameter selection in cycle 3: nr = 13

gp	1	2	3	4	5	6	7	0	0	0	0						
pp	8	9	10	0	0	0	11	12	13	0	0	0	0	0	0	0	0
tp	14	0															
sp	0	0	0	0	0		0	0	0	0	0		0	0	0	0	0
pp	15	15	16	0	0	0	17	18	19	0	0	0	0	0	0	0	0

```
tp  20   0
sp   0   0   0   0   0       0   0   0   0   0
pp  21  21  22   0   0   0  23  24  25   0   0   0   0   0   0   0   0
tp  26   0
sp   0   0   0   0   0       0   0   0   0   0
```

L.S.	Ncyl	Nobs	Npar	Nvar	Rp	Rwp	Rp"	Re	GOF
Before cyl	3	4751	4467	26	0.27135	0.32692	0.55761	0.03762	8.690

Comp	Nref	SumIo	: SumIc	SumdI	RBragg	RF
1	147	1.00000	0.74724	0.25276	0.34456	0.18230

Comp	Nref	SumIo	: SumIc	SumdI	RBragg	RF
2	26	1.00000	0.72884	0.27116	0.31499	0.14966

Comp	Nref	SumIo	: SumIc	SumdI	RBragg	RF
3	35	1.00000	0.92182	0.07818	0.18057	0.11704

Change of l.s. parameters in cycle 3

Com.	Atoms	Para	old	change	new	e.s.d.	
		b0	3.106388	-0.539113	2.567275	0.052659	>5%
		b1	-3.378353	0.671537	-2.706817	0.181501	>5%
		b2	0.892862	0.234557	1.127420	0.295282	>5%
		b3	0.765908	-0.899671	-0.133762	0.709028	>5%
		b4	-0.931423	0.242773	-0.688650	0.318413	>5%
		b5	1.203531	0.084641	1.288172	0.617270	>5%
		t0	-0.008390	0.001696	-0.006694	0.003983	>5%
1		a	9.166616	0.001881	9.168497	0.002043	>5%
1		b	5.440846	-0.002898	5.437948	0.001140	>5%
1		c	5.145334	0.004513	5.149848	0.000962	>5%
1		U	0.097200	0.096021	0.145210	0.091628	>5%
1		V	-0.033300	0.193215	0.063307	0.095075	>5%
1		W	0.072000	0.066384	0.105192	0.021632	>5%
1		Scale	4.313642	1.741704	6.055346	0.094058	>5%

2	a	3.789772	0.001160	3.790931	0.000631	>5%
2	b	3.789772	0.001160	3.790931	0.000000	
2	c	9.505519	-0.006873	9.498646	0.002253	>5%
2	U	0.097200	0.186335	0.190367	0.114570	>5%
2	V	-0.033300	0.016050	-0.025275	0.114807	>5%
2	W	0.072000	0.145061	0.144530	0.024457	>5%
2	Scale	1.838878	0.678017	2.516896	0.060451	>5%
3	a	4.759533	0.000737	4.760271	0.000345	>5%
3	b	4.759533	0.000737	4.760271	0.000000	
3	c	12.992633	0.002831	12.995464	0.001296	>5%
3	U	0.010800	0.006684	0.014142	0.013893	>5%
3	V	-0.003700	0.003578	-0.001911	0.017000	>5%
3	W	0.008000	0.005495	0.010748	0.004908	>5%
3	Scale	2.363253	0.480222	2.843475	0.066772	>5%

Lp correction (normal): A part = 1.000 B part = 0.790

Parameter selection in cycle 4: nr = 12

```
gp   1   2   3   4   5   6   7   0   0   0   0
pp   8   9  10   0   0   0  11  12  13   0   0   0   0   0   0   0   0
tp  14   0
sp   0   0   0   0   0       0   0   0   0   0       0   0   0   0   0

pp  15  15  16   0   0   0  17  18  19   0   0   0   0   0   0   0   0
tp  20   0
sp   0   0   0   0   0       0   0   0   0   0
pp  21  21  22   0   0   0  23  24  25   0   0   0   0   0   0   0   0
tp  26   0
sp   0   0   0   0   0       0   0   0   0   0
```

L.S.	Ncyl	Nobs	Npar	Nvar	Rp	Rwp	Rp"	Re	GOF
Before cyl	4	4751	4510	26	0.21660	0.26624	0.39320	0.03762	7.077

Comp	Nref	SumIo : SumIc	SumdI	RBragg	RF

Comp	Nref	SumIo	SumIc	SumdI	RBragg	RF
1	152	1.00000	0.92928	0.07072	0.19312	0.10382

Comp	Nref	SumIo	SumIc	SumdI	RBragg	RF
2	26	1.00000	0.91176	0.08824	0.15913	0.08142

Comp	Nref	SumIo	SumIc	SumdI	RBragg	RF
3	36	1.00000	1.01569	-0.01569	0.10936	0.07618

Change of l.s. parameters in cycle 4

Com.	Atoms	Para	old	change	new	e.s.d.	
		b0	2.567275	-0.373619	2.193657	0.043953	>5%
		b1	-2.706817	0.477951	-2.228866	0.148831	>5%
		b2	1.127420	0.024016	1.151435	0.241076	>5%
		b3	-0.133762	-0.538778	-0.672541	0.579208	>5%
		b4	-0.688650	0.325494	-0.363156	0.260170	>5%
		b5	1.288172	-0.038529	1.249643	0.503843	>5%
		t0	-0.006694	0.008553	0.001859	0.003586	>5%
1		a	9.168497	0.003556	9.172053	0.001914	>5%
1		b	5.437948	-0.000288	5.437660	0.001048	>5%
1		c	5.149848	0.005356	5.155203	0.000876	>5%
1		U	0.145210	0.197266	0.243843	0.121709	>5%
1		V	0.063307	0.248201	0.187408	0.125118	>5%
1		W	0.105192	0.084887	0.147636	0.028192	>5%
1		Scale	6.055346	1.057742	7.113088	0.089408	>5%
2		a	3.790931	0.000770	3.791702	0.000609	>5%
2		b	3.790931	0.000770	3.791702	0.000000	
2		c	9.498646	-0.005797	9.492849	0.002149	>5%
2		U	0.190367	0.395051	0.387893	0.165455	>5%
2		V	-0.025275	-0.059057	-0.054804	0.164398	>5%
2		W	0.144530	0.220054	0.254557	0.034906	>5%
2		Scale	2.516896	0.336399	2.853295	0.057486	>5%
3		a	4.760271	0.000962	4.761232	0.000318	>5%
3		b	4.760271	0.000962	4.761232	0.000000	
3		c	12.995464	0.002977	12.998442	0.001212	>5%

```
     3            U    0.014142    0.013511    0.020897    0.015591 >5%
     3            V   -0.001911   -0.008930   -0.006376    0.019074 >5%
     3            W    0.010748    0.009196    0.015346    0.005477 >5%
     3        Scale    2.843475    0.127917    2.971392    0.056977 >5%


  Lp correction (normal):  A part =   1.000  B part =   0.790

------------------------------------------------------------------------
  Parameter selection in cycle  5:  nr = 11
  gp   1   2   3   4   5   6   7   0   0   0   0
  pp   8   9  10   0   0   0  11  12  13  14  15  16   0   0   0   0   0
  tp  17   0
  sp   0   0   0   0   0       0   0   0   0   0       0   0   0   0   0

  pp  18  18  19   0   0   0  20  21  22  14  15  16   0   0   0   0   0
  tp  23   0
  sp   0   0   0   0   0       0   0   0   0   0
  pp  24  24  25   0   0   0  26  27  28  14  15  16   0   0   0   0   0
  tp  29   0
  sp   0   0   0   0   0       0   0   0   0   0

  L.S.       Ncyl Nobs Npar Nvar       Rp     Rwp     Rp"      Re     GOF
  Before cyl    5 4751 4527   29  0.17040 0.21602 0.28485 0.03761   5.744

            Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
               1  157            1.00000 0.99157 0.00843 0.14296 0.07599

            Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
               2   26            1.00000 0.97962 0.02038 0.10404 0.05983

            Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
               3   37            1.00000 1.01645-0.01645 0.06406 0.04929

  Change of l.s. parameters in cycle  5
   Com.  Atoms  Para         old      change         new      e.s.d.
```

	b0	2.193657	-0.259345	1.934312	0.036486	>5%
	b1	-2.228866	0.297023	-1.931843	0.122303	>5%
	b2	1.151435	-0.021046	1.130389	0.196504	>5%
	b3	-0.672541	-0.058237	-0.730778	0.474374	>5%
	b4	-0.363156	0.280303	-0.082853	0.212345	>5%
	b5	1.249643	-0.373102	0.876541	0.412453	>5%
	t0	0.001859	-0.035112	-0.033253	0.005327	>5%
1	a	9.172053	0.003644	9.175698	0.002158	>5%
1	b	5.437660	0.003091	5.440750	0.001261	>5%
1	c	5.155203	0.003296	5.158500	0.001019	>5%
1	U	0.243843	0.613331	0.550509	0.155995	>5%
1	V	0.187408	-0.288915	0.042950	0.160538	>5%
1	W	0.147636	0.251633	0.273452	0.035910	>5%
1	a0	1.180000	-0.330571	1.014715	0.104438	>5%
1	a1	-0.110000	-0.946963	-0.583482	0.207068	>5%
1	a2	-0.028000	0.230403	0.087201	0.031296	>5%
1	Scale	7.113088	0.416033	7.529121	0.081996	>5%
2	a	3.791702	0.000321	3.792023	0.000801	>5%
2	b	3.791702	0.000321	3.792023	0.000000	
2	c	9.492849	-0.007007	9.485843	0.002551	>5%
2	U	0.387893	0.758671	0.767229	0.250414	>5%
2	V	-0.054804	-0.064014	-0.086811	0.243636	>5%
2	W	0.254557	0.308634	0.408874	0.050747	>5%
2	a0	1.180000	-0.330571	1.014715	0.000000	
2	a1	-0.110000	-0.946963	-0.583482	0.000000	
2	a2	-0.028000	0.230403	0.087201	0.000000	
2	Scale	2.853295	0.526731	3.380025	0.054829	>5%
3	a	4.761232	-0.001721	4.759512	0.000445	>5%
3	b	4.761232	-0.001721	4.759512	0.000000	
3	c	12.998442	-0.005117	12.993325	0.001498	>5%
3	U	0.020897	0.052512	0.047153	0.016975	>5%
3	V	-0.006376	-0.064495	-0.038623	0.020838	>5%
3	W	0.015346	0.026628	0.028660	0.005970	>5%
3	a0	1.180000	-0.330571	1.014715	0.000000	

```
    3           a1   -0.110000    -0.946963    -0.583482     0.000000
    3           a2   -0.028000     0.230403     0.087201     0.000000
    3        Scale    2.971392     0.074998     3.046390     0.047749 >5%


 Lp correction (normal):  A part =   1.000  B part =   0.790

-----------------------------------------------------------------------
 Parameter selection in cycle  6:  nr = 10
 gp   1   2   3   4   5   6   7   0   0   0   0
 pp   8   9  10   0   0   0  11  12  13  14  15  16  17   0  18   0   0
 tp  19   0
 sp   0   0   0   0   0       0   0   0   0   0       0   0   0   0   0

 pp  20  20  21   0   0   0  22  23  24  14  15  16  17   0  18   0   0
 tp  25   0
 sp   0   0   0   0   0       0   0   0   0   0
 pp  26  26  27   0   0   0  28  29  30  14  15  16  17   0  18   0   0
 tp  31   0
 sp   0   0   0   0   0       0   0   0   0   0

 L.S.       Ncyl Nobs Npar Nvar       Rp      Rwp      Rp"       Re      GOF
 Before cyl    6 4751 4551   31  0.12682 0.16370 0.20086 0.03760    4.354

           Comp Nref              SumIo : SumIc   SumdI  RBragg       RF
              1  158            1.00000 1.02143-0.02143 0.10106 0.05637

           Comp Nref              SumIo : SumIc   SumdI  RBragg       RF
              2   26            1.00000 1.01960-0.01960 0.09921 0.05721

           Comp Nref              SumIo : SumIc   SumdI  RBragg       RF
              3   37            1.00000 1.01466-0.01466 0.03019 0.03057

 Change of l.s. parameters in cycle  6
  Com.  Atoms  Para         old      change         new      e.s.d.
```

	b0	1.934312	-0.552461	1.381851	0.030817	>5%
	b1	-1.931843	0.906080	-1.025763	0.096855	>5%
	b2	1.130389	-0.655569	0.474820	0.150983	>5%
	b3	-0.730778	0.060219	-0.670559	0.362647	>5%
	b4	-0.082853	1.268721	1.185868	0.165420	>5%
	b5	0.876541	-1.176641	-0.300099	0.316028	>5%
	t0	-0.033253	-0.018607	-0.051860	0.004728	>5%
1	a	9.175698	-0.006231	9.169467	0.002036	>5%
1	b	5.440750	0.001153	5.441903	0.001210	>5%
1	c	5.158500	0.000377	5.158876	0.000986	>5%
1	U	0.550509	0.140444	0.620731	0.180912	>5%
1	V	0.042950	0.118218	0.102059	0.183879	>5%
1	W	0.273452	0.037961	0.292433	0.041332	>5%
1	a0	1.014715	0.143836	1.086633	0.077886	>5%
1	a1	-0.583482	0.257726	-0.454619	0.125208	>5%
1	a2	0.087201	-0.030429	0.071987	0.018423	>5%
1	e/mL0	0.500000	0.532200	0.766100	0.029171	>5%
1	e/mH0	0.500000	0.773057	0.886529	0.033603	>5%
1	Scale	7.529121	1.451883	8.981004	0.080686	>5%
2	a	3.792023	-0.001556	3.790467	0.000808	>5%
2	b	3.792023	-0.001556	3.790467	0.000000	
2	c	9.485843	-0.014208	9.471635	0.002460	>5%
2	U	0.767229	1.472331	1.503394	0.343819	>5%
2	V	-0.086811	-0.381682	-0.277652	0.325541	>5%
2	W	0.408874	0.191509	0.504629	0.066580	>5%
2	a0	1.014715	0.143836	1.086633	0.000000	
2	a1	-0.583482	0.257726	-0.454619	0.000000	
2	a2	0.087201	-0.030429	0.071987	0.000000	
2	e/mL0	0.500000	0.532200	0.766100	0.000000	
2	e/mH0	0.500000	0.773057	0.886529	0.000000	
2	Scale	3.380025	0.751217	4.131242	0.048745	>5%
3	a	4.759512	-0.001396	4.758116	0.000379	>5%
3	b	4.759512	-0.001396	4.758116	0.000000	
3	c	12.993325	-0.003822	12.989503	0.001295	>5%
3	U	0.047153	-0.044991	0.024657	0.017420	>5%

```
    3            V   -0.038623     0.069613    -0.003817     0.021173 >5%
    3            W    0.028660    -0.024951     0.016184     0.006096 >5%
    3           a0    1.014715     0.143836     1.086633     0.000000
    3           a1   -0.583482     0.257726    -0.454619     0.000000
    3           a2    0.087201    -0.030429     0.071987     0.000000
    3        e/mL0    0.550000     0.532200     0.816100     0.000000
    3        e/mH0    0.550000     0.773057     0.936529     0.000000
    3        Scale    3.046390     0.482632     3.529022     0.039355 >5%


 Lp correction (normal):  A part =   1.000  B part =   0.790

-------------------------------------------------------------------------
 Parameter selection in cycle  7:  nr =  9
 gp   1   2   3   4   5   6   7   0   0   0   0
 pp   8   9  10   0   0   0  11  12  13  14  15  16  17  18  19  20   0
 tp  21   0
 sp   0   0   0   0   0       0   0   0   0   0       0   0   0   0   0

 pp  22  22  23   0   0   0  24  25  26  14  15  16  17  18  19  20   0
 tp  27   0
 sp   0   0   0   0   0       0   0   0   0   0
 pp  28  28  29   0   0   0  30  31  32  14  15  16  17  18  19  20   0
 tp  33   0
 sp   0   0   0   0   0       0   0   0   0   0

 L.S.       Ncyl Nobs Npar Nvar       Rp      Rwp      Rp"       Re      GOF
 Before cyl    7 4751 4557   33  0.09268 0.11581 0.12985 0.03759    3.081

           Comp Nref             SumIo : SumIc   SumdI  RBragg       RF
              1  158            1.00000 1.08117-0.08117 0.08868 0.06072

           Comp Nref             SumIo : SumIc   SumdI  RBragg       RF
              2   26            1.00000 1.09641-0.09641 0.09781 0.06841

           Comp Nref             SumIo : SumIc   SumdI  RBragg       RF
```

3 37 1.00000 1.05890-0.05890 0.06110 0.04246

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Change of l.s. parameters in cycle 14

Com.	Atoms	Para	old	change	new	e.s.d.	
		b0	1.460997	0.000976	1.461973	0.018759	>5%
		b1	-0.964973	-0.001862	-0.966835	0.039174	
		b2	0.018860	-0.000835	0.018025	0.077047	
		b3	0.026014	0.004456	0.030470	0.154850	
		b4	1.690182	-0.000080	1.690102	0.078158	
		b5	-1.045206	-0.003102	-1.048307	0.138383	
		t0	-0.050607	0.000015	-0.050591	0.001882	
1		a	9.169816	-0.000066	9.169750	0.001191	>5%
1		b	5.445023	-0.000065	5.444958	0.000728	>5%
1		c	5.160255	-0.000084	5.160172	0.000610	>5%
1		U	1.086726	0.022721	1.098087	0.159413	>5%
1		V	-0.248553	-0.017861	-0.257483	0.157538	>5%
1		W	0.545681	0.008226	0.549794	0.035490	>5%
1		a0	1.086800	0.026676	1.100138	0.047408	>5%
1		a1	-0.294907	0.012314	-0.288750	0.053222	>5%
1		a2	0.050915	-0.001174	0.050328	0.007296	>5%
1		e/mL0	0.837979	0.004263	0.840110	0.025307	>5%
1		e/mL1	-0.000454	-0.000368	-0.000638	0.000653	>5%
1		e/mH0	0.896335	0.005192	0.898931	0.025122	>5%
1		e/mH1	-0.000613	-0.000040	-0.000633	0.000674	>5%
1		Scale	9.192083	-0.002512	9.189571	0.055813	
1		Temp	0.452711	0.000900	0.453610	0.029960	
2		a	3.790296	-0.000100	3.790196	0.000694	>5%
2		b	3.790296	-0.000100	3.790196	0.000000	
2		c	9.443354	-0.000232	9.443121	0.002106	>5%
2		U	2.812092	-0.114003	2.755091	0.502845	>5%

2	V	1.318585	0.207962	1.422566	0.452687	>5%
2	W	0.403233	-0.038455	0.384005	0.087185	>5%
2	a0	1.086800	0.026676	1.100138	0.000000	
2	a1	-0.294907	0.012314	-0.288750	0.000000	
2	a2	0.050915	-0.001174	0.050328	0.000000	
2	e/mL0	0.837979	0.004263	0.840110	0.000000	
2	e/mL1	-0.000454	-0.000368	-0.000638	0.000000	
2	e/mH0	0.896335	0.005192	0.898931	0.000000	
2	e/mH1	-0.000613	-0.000040	-0.000633	0.000000	
2	Scale	4.683733	0.000790	4.684522	0.029185	
2	Temp	0.452711	0.000900	0.453610	0.000000	
3	a	4.758222	-0.000010	4.758212	0.000171	>5%
3	b	4.758222	-0.000010	4.758212	0.000000	
3	c	12.989905	-0.000021	12.989884	0.000580	
3	U	-0.006214	-0.000506	-0.006467	0.007408	>5%
3	V	0.035713	0.000924	0.036174	0.009020	>5%
3	W	0.009051	-0.000116	0.008994	0.002446	
3	a0	1.086800	0.026676	1.100138	0.000000	
3	a1	-0.294907	0.012314	-0.288750	0.000000	
3	a2	0.050915	-0.001174	0.050328	0.000000	
3	e/mL0	0.887979	0.004263	0.890110	0.000000	
3	e/mL1	-0.000454	-0.000368	-0.000638	0.000000	
3	e/mH0	0.946335	0.005192	0.948931	0.000000	
3	e/mH1	-0.000613	-0.000040	-0.000633	0.000000	
3	Scale	3.667836	-0.000131	3.667705	0.023781	
3	Temp	0.452711	0.000900	0.453610	0.000000	

Lp correction (normal): A part = 1.000 B part = 0.790

Parameter selection in cycle 15: nr = 1

gp	1	2	3	4	5	6	7	0	0	0	0						
pp	8	9	10	0	0	0	11	12	13	14	15	16	17	18	19	20	0
tp	21	22															
sp	0	0	0	0	0		0	0	0	0	0		0	0	0	0	0

```
pp  23  23  24   0   0   0  25  26  27  14  15  16  17  18  19  20   0
tp  28  22
sp   0   0   0   0   0       0   0   0   0   0
pp  29  29  30   0   0   0  31  32  33  14  15  16  17  18  19  20   0
tp  34  22
sp   0   0   0   0   0       0   0   0   0   0



 Rwp factor dose not change.

 L.S.       Ncyl Nobs Npar Nvar       Rp     Rwp     Rp"      Re     GOF
 Rwp =const   15 4751 4588   34  0.04852 0.06182 0.06842 0.03759   1.645

           Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
              1  158            1.00000 1.06520-0.06520 0.06886 0.04522

           Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
              2   26            1.00000 1.09320-0.09320 0.09320 0.05509

           Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
              3   37            1.00000 1.02378-0.02378 0.02896 0.02349

 .-------------------------------------------------------------.
 ¦ You can see the pattern by entering "disp" in another window. ¦
  -------------------------------------------------------------

 Enter option:
  -1: go back to upper menu
   0: terminate l.s. cycles
   1: continue  l.s. cycles
   2: display refined parameters & go back to this menu
1
```

```
  Select:
    0: refine structural parameters from next cycles
    1: no refinement of structural parameters
1

  The number of cycles remained = 25

  Select a mode of refinement:
    -3: terminate/pause l.s. cycles
    -2: full-manual (single-step)
    -1: manual
     0: automatic
     n: repeat n times (n >= 1)
-2

--------------- Parameter selection for the L.S. of cycle 16 -----------


 Global parameters:

  For parameters:    b0,    b1,    b2,    b3,    b4,    b5,
1 1 1 1 1 1
  For parameters:    t0,    t1,    t2,    t3,
1 0 0 0
  For parameters:     E,
0

 Profile parameters:


  For 1th component:
  For parameters:     a,     b,     c, alpha,  beta, gamma,
1
  For parameters:     U,     V,     W,
1 1 1
  For parameters:    a0,    a1,    a2,
```

1 1 1
  For parameters: e/mL0, e/mL1,
1 1
  For parameters: e/mH0, e/mH1,
1 1

  For 2th component:
  For parameters: a,   b,   c, alpha, beta, gamma,
1
  For parameters: U,   V,   W,
1 1 1
  For parameters: a0,   a1,   a2,
1 1 1
  For parameters: e/mL0, e/mL1,
1 1
  For parameters: e/mH0, e/mH1,
1 1

  For 3th component:
  For parameters: a,   b,   c, alpha, beta, gamma,
1
  For parameters: U,   V,   W,
1 1 1
  For parameters: a0,   a1,   a2,
1 1 1
  For parameters: e/mL0, e/mL1,
1 1
  For parameters: e/mH0, e/mH1,
1 1

  Scale and OATM parameters:

  For 1th component:
  For parameters: Scale, Temp,
1 1

For 2th component:
For parameters: Scale, Temp,
1 2

For 3th component:
For parameters: Scale, Temp,
1 2

Texture parameters:

Structural paremeters:

For 1th component:
For parameters: alpha, x, y, z, Biso, of Ti1
0 0 0 0 0 0 0

For 1th component:
For parameters: alpha, x, y, z, Biso, of O1
0 0 0 0 0 0 0

For 1th component:
For parameters: alpha, x, y, z, Biso, of O2
0 0 0 0 0 0 0

For 2th component:
For parameters: alpha, x, y, z, Biso, of Ti1
0 0 0 0 0 0 0

For 2th component:
For parameters: alpha, x, y, z, Biso, of O1
0 0 0 0 0 0 0

For 3th component:

```
  For parameters: alpha,     x,     y,     z,  Biso,  of All
0 0 0 0 0 0 0

  For 3th component:
  For parameters: alpha,     x,     y,     z,  Biso,  of O1
0 0 0 0 0 0 0

  How many cycles do you repeat this selectoin ?
    -1: back to the beginning of selection
     0: to parameter convergence
     n: n cycles
0

  Lp correction (normal):  A part =   1.000  B part =   0.790

-------------------------------------------------------------------------
  Parameter selection in cycle 16:  nr =  0
  gp   1   2   3   4   5   6   7   0   0   0   0
  pp   8   9  10   0   0   0  11  12  13  14  15  16  17  18  19  20   0
  tp  21  22
  sp   0   0   0   0   0       0   0   0   0   0       0   0   0   0   0

  pp  23  23  24   0   0   0  25  26  27  28  29  30  31  32  33  34   0
  tp  35  22
  sp   0   0   0   0   0       0   0   0   0   0
  pp  36  36  37   0   0   0  38  39  40  41  42  43  44  45  46  47   0
  tp  48  22
  sp   0   0   0   0   0       0   0   0   0   0

  L.S.       Ncyl Nobs Npar Nvar       Rp     Rwp     Rp"      Re     GOF
  Before cyl  16 4751 4588   48  0.04852 0.06182 0.06842 0.03753   1.647

            Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
               1  158           1.00000 1.06520-0.06520 0.06886 0.04522

            Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
```

```
    2   26            1.00000 1.09320-0.09320 0.09320 0.05509

  Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
    3   37            1.00000 1.02378-0.02378 0.02896 0.02349
```

＃＃

途中省略

＃＃

```
 Rwp factor dose not change.

 L.S.       Ncyl Nobs Npar Nvar       Rp     Rwp     Rp"      Re     GOF
 Rwp =const  22 4751 4582   48  0.04564 0.05890 0.06541 0.03753   1.569

          Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
            1  158            1.00000 1.06055-0.06055 0.06505 0.03798

          Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
            2   26            1.00000 1.06859-0.06859 0.06859 0.04125

          Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
            3   37            1.00000 1.02444-0.02444 0.03047 0.02338

 .-------------------------------------------------------------.
 ¦ You can see the pattern by entering "disp" in another window. ¦
  -------------------------------------------------------------

 Enter option:
  -1: go back to upper menu
   0: terminate l.s. cycles
   1: continue  l.s. cycles
   2: display refined parameters & go back to this menu
```

0 ←ダンピングファクターを１に戻して精密化を継続するために、一旦、最小二乗サイクルを終了します。

```
  Select:
    0: transfer overall temperature factor to individual ones
    1: no transferring
1


--------------- Output profile and strutural parameters ---------

  Select a file name for profile parameters
   -1:no output,   0:file A,   1:file B,   2:file C,   3:your option.
-1  ←プロファイルパラメータは解析途中なので、ここでは出力しません。

  Select a filename for strutural parameters:
   -1:no output,   0:file A,   1:file B,   2:file C,   3:your option.
-1  ←構造パラメータは解析途中なので、ここでは出力しません。

  Select:
    0: continue refinement
    1: change the 2theta-range to be analyzed
    2: read new profile/structural parameters
    3: read a new intensity data set
    4: terminate job
0  ←精密化を継続します。


--------------- Correction of parameters before the l.s. ---------------

   -1: terminate job (results will be aborted)
    0: no change
    1: correct global and profile parameters
    2: correct structural parameters
    3: correct scale, OATM, or texture parameters
    4: see the pattern before the l.s.
    5: how to change parameter values ?
0
```

```
-------------- Set calculation conditions ----------------------------

  Calculation of profile function is truncated
  when profile intensity < Y(lim) (unit = counts).

  Damping factors (DF) will be applied when parameters
  oscillate or are apt to diverge during the least-squares.

  Y(lim)  D.F.  bj    tj  I2I1  Cell  FWHM  Ae/m axyzB  Scal  OATM  Xtex
     1.5      1.00  1.00  1.00  1.00  0.50  0.50  1.00  1.00  1.00  1.00


  Enter number to change parameters:
    0: no change,   1: Y(lim),   2: D.F.
2  ←ダンピングファクターを１に戻すので、変更を指定します。

  Input D.F. (default = 1.0) for
    bj, tj, E, cell, FWHM, Ae/m, axyzB, Scale, OATM, Xtex.
1 1 1 1 1 1 1 1 1 1  ←すべてのダンピングファクターを１にします。

  Y(lim)  D.F.  bj    tj  I2I1  Cell  FWHM  Ae/m axyzB  Scal  OATM  Xtex
     1.5      1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00


  Enter number to change parameters:
    0: no change,   1: Y(lim),   2: D.F.
0

-------------- Optimization was started ------------------------------

  Select a mode of refinement:
    -3: terminate/pause l.s. cycles
    -2: full-manual (single-step)
    -1: manual
```

```
     0: automatic
-2

--------------- Parameter selection for the L.S. of cycle  1 -----------


 Global parameters:

  For parameters:    b0,    b1,    b2,    b3,    b4,    b5,
1 1 1 1 1 1
  For parameters:    t0,    t1,    t2,    t3,
1 0 0 0 0
  For parameters:     E,
0

 Profile parameters:


  For 1th component:
  For parameters:     a,     b,     c, alpha,  beta, gamma,
1
  For parameters:     U,     V,     W,
1 1 1
  For parameters:    a0,    a1,    a2,
1 1 1
  For parameters: e/mL0, e/mL1,
1 1
  For parameters: e/mH0, e/mH1,
1 1

  For 2th component:
  For parameters:     a,     b,     c, alpha,  beta, gamma,
1
  For parameters:     U,     V,     W,
1 1 1
  For parameters:    a0,    a1,    a2,
```

1 1 1
  For parameters: e/mL0, e/mL1,
1 1
  For parameters: e/mH0, e/mH1,
1 1

  For 3th component:
  For parameters: a,   b,   c, alpha, beta, gamma,
1
  For parameters: U,   V,   W,
1 1 1
  For parameters: a0,   a1,   a2,
1 1 1
  For parameters: e/mL0, e/mL1,
1 1
  For parameters: e/mH0, e/mH1,
1 1

  Scale and OATM parameters:

  For 1th component:
  For parameters: Scale, Temp,
1 1

  For 2th component:
  For parameters: Scale, Temp,
1 2

  For 3th component:
  For parameters: Scale, Temp,
1 2

  Texture parameters:

Structural paremeters:

For 1th component:
For parameters: alpha, x, y, z, Biso, of Ti1
0 0 0 0 0 0 0

For 1th component:
For parameters: alpha, x, y, z, Biso, of O1
0 0 0 0 0 0 0

For 1th component:
For parameters: alpha, x, y, z, Biso, of O2
0 0 0 0 0 0 0

For 2th component:
For parameters: alpha, x, y, z, Biso, of Ti1
0 0 0 0 0 0 0

For 2th component:
For parameters: alpha, x, y, z, Biso, of O1
0 0 0 0 0 0 0

For 3th component:
For parameters: alpha, x, y, z, Biso, of Al1
0 0 0 0 0 0 0

For 3th component:
For parameters: alpha, x, y, z, Biso, of O1
0 0 0 0 0 0 0

How many cycles do you repeat this selectoin ?
-1: back to the beginning of selection
0: to parameter convergence
n: n cycles
0

```
 Lp correction (normal):  A part =   1.000  B part =   0.790

-------------------------------------------------------------------------
 Parameter selection in cycle  1:  nr =  0
 gp   1   2   3   4   5   6   7   0   0   0   0
 pp   8   9  10   0   0   0  11  12  13  14  15  16  17  18  19  20   0
 tp  21  22
 sp   0   0   0   0   0       0   0   0   0   0       0   0   0   0   0

 pp  23  23  24   0   0   0  25  26  27  28  29  30  31  32  33  34   0
 tp  35  22
 sp   0   0   0   0   0       0   0   0   0   0
 pp  36  36  37   0   0   0  38  39  40  41  42  43  44  45  46  47   0
 tp  48  22
 sp   0   0   0   0   0       0   0   0   0   0

 L.S.       Ncyl Nobs Npar Nvar       Rp     Rwp     Rp"      Re      GOF
 Before cyl    1 4751 4582   48  0.04559 0.05885 0.06535 0.03753   1.568

           Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
              1  158            1.00000 1.06146-0.06146 0.06576 0.03843

           Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
              2   26            1.00000 1.06820-0.06820 0.06820 0.04098

           Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
              3   37            1.00000 1.02464-0.02464 0.03104 0.02371

 Change of l.s. parameters in cycle  1
  Com.  Atoms  Para         old      change         new      e.s.d.

                b0    1.603730    0.005071    1.608801    0.018830 >5%
                b1   -0.954094    0.017695   -0.936400    0.038698 >5%
                b2   -0.446076   -0.005313   -0.451389    0.076511 >5%
                b3    0.318316   -0.060276    0.258041    0.151863 >5%
```

	b4	2.116148	0.001439	2.117587	0.077889	
	b5	-1.338314	0.047388	-1.290926	0.135793	>5%
	t0	-0.036756	-0.000010	-0.036766	0.003987	
1	a	9.178926	-0.000301	9.178624	0.001623	>5%
1	b	5.449558	0.000010	5.449569	0.000936	
1	c	5.164395	-0.000011	5.164384	0.000837	
1	U	1.350934	-0.023130	1.327804	0.158815	>5%
1	V	-0.355703	0.026869	-0.328834	0.157735	>5%
1	W	0.529450	-0.005709	0.523741	0.037714	>5%
1	a0	0.939880	0.016943	0.956824	0.059048	>5%
1	a1	0.010042	0.022407	0.032449	0.095660	>5%
1	a2	-0.011381	-0.003243	-0.014624	0.015873	>5%
1	e/mL0	1.057688	0.008399	1.066087	0.046142	>5%
1	e/mL1	-0.002323	-0.000300	-0.002623	0.001180	>5%
1	e/mH0	1.184654	0.006831	1.191485	0.048599	>5%
1	e/mH1	-0.009845	-0.000136	-0.009981	0.001198	>5%
1	Scale	9.517640	-0.014142	9.503498	0.061572	>5%
1	Temp	0.725165	0.005099	0.730264	0.032689	>5%
2	a	3.785971	-0.000084	3.785887	0.001174	>5%
2	b	3.785971	-0.000084	3.785887	0.000000	
2	c	9.432652	-0.000229	9.432424	0.003211	>5%
2	U	1.418582	-0.165096	1.253486	0.614760	>5%
2	V	3.156249	0.019296	3.175545	0.509504	
2	W	0.157086	0.014078	0.171164	0.104896	>5%
2	a0	1.556241	0.071909	1.628150	0.143253	>5%
2	a1	-0.408279	0.046104	-0.362175	0.162097	>5%
2	a2	0.092438	-0.004366	0.088072	0.022747	>5%
2	e/mL0	0.837025	-0.014124	0.822901	0.050998	>5%
2	e/mL1	-0.010956	-0.000058	-0.011014	0.001452	
2	e/mH0	0.676354	-0.027675	0.648679	0.059346	>5%
2	e/mH1	0.007138	0.000869	0.008007	0.001565	>5%
2	Scale	4.535686	0.008931	4.544618	0.032604	>5%
2	Temp	0.725165	0.005099	0.730264	0.000000	
3	a	4.759271	0.000001	4.759272	0.000327	
3	b	4.759271	0.000001	4.759272	0.000000	

3	c	12.992382	-0.000011	12.992371	0.000922	
3	U	-0.007063	0.000041	-0.007022	0.006183	
3	V	0.023971	-0.000701	0.023269	0.008373	>5%
3	W	0.012392	0.000316	0.012708	0.002722	>5%
3	a0	0.843420	-0.005018	0.838402	0.108183	
3	a1	-0.681517	0.010367	-0.671149	0.220128	
3	a2	0.074624	-0.003676	0.070948	0.031931	>5%
3	e/mL0	0.699164	-0.013572	0.685592	0.103250	>5%
3	e/mL1	0.005675	0.000271	0.005946	0.001995	>5%
3	e/mH0	1.177233	0.004128	1.181361	0.127854	
3	e/mH1	-0.003618	-0.000098	-0.003716	0.002258	
3	Scale	3.892279	0.001205	3.893484	0.027702	
3	Temp	0.725165	0.005099	0.730264	0.000000	

Lp correction (normal): A part = 1.000 B part = 0.790

L.S.	Ncyl	Nobs	Npar	Nvar	Rp	Rwp	Rp"	Re	GOF
Before cyl	2	4751	4582	48	0.04561	0.05884	0.06543	0.03753	1.568

Comp	Nref	SumIo	:	SumIc	SumdI	RBragg	RF
1	158	1.00000	1.06074	-0.06074	0.06514	0.03794	

Comp	Nref	SumIo	:	SumIc	SumdI	RBragg	RF
2	26	1.00000	1.06883	-0.06883	0.06883	0.04170	

Comp	Nref	SumIo	:	SumIc	SumdI	RBragg	RF
3	37	1.00000	1.02459	-0.02459	0.03034	0.02358	

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Rwp factor dose not change.

```
  L.S.       Ncyl Nobs Npar Nvar       Rp     Rwp     Rp"      Re     GOF
  Rwp =const    4 4751 4582   48  0.04556 0.05883 0.06539 0.03753   1.568

            Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
               1  158            1.00000 1.06096-0.06096 0.06531 0.03811

            Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
               2   26            1.00000 1.06899-0.06899 0.06899 0.04231

            Comp Nref             SumIo : SumIc   SumdI  RBragg      RF
               3   37            1.00000 1.02489-0.02489 0.03049 0.02393

  .-------------------------------------------------------------.
  ¦ You can see the pattern by entering "disp" in another window. ¦
   -------------------------------------------------------------

  Enter option:
   -1: go back to upper menu
    0: terminate l.s. cycles
    1: continue  l.s. cycles
    2: display refined parameters & go back to this menu
0

  Select:
    0: transfer overall temperature factor to individual ones
    1: no transferring
1


--------------- Output profile and strutural parameters ---------

  Select a file name for profile parameters
   -1:no output,   0:file A,   1:file B,   2:file C,   3:your option.
2
```

```
  Profile parameters were written on  a file: reflexc.d

  Select a filename for strutural parameters:
   -1:no output,   0:file A,   1:file B,   2:file C,   3:your option.
2

  Atomic parameters were written on datafile: atomsc.d

  Select:
    0: continue refinement
    1: change the 2theta-range to be analyzed
    2: read new profile/structural parameters
    3: read a new intensity data set
    4: terminate job
4
  File name for printed output is /tmp/pfls.txt

c:¥xbin>
```