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     Archiving SAFE_NEUTRON_FINAL_STEPHANSS.EXP as SAFE_NEUTRON_FINAL_STEPHANSS.O01
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1SFO                                                                    Version        Jun 14 18:25:39 2011
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           |-----------------------------------------------------------|
           |              Program POWPREF Version MacOSX               |
           | Prepares powder histograms for least-squares refinement   |
           |         Distributed on Wed Apr 21 18:37:06 2010           |
           |-----------------------------------------------------------|

        |-------------------------------------------------------------|
        |            Allen C. Larson and Robert B. Von Dreele         |
        |      Manuel Lujan, Jr. Neutron Scattering Center, MS-H805   |
        |      Los Alamos National Laboratory, Los Alamos, NM  87545  |
        |                                                             |
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        |-------------------------------------------------------------|

 The last history record is :
     HSTRY 83 EXPGUI 1113 1033 (1 changes) -- 06/14/2011 18:25:16
 Data for bank  1 read from file e56881.gsa
 The powder pattern has  4524 channels with   1 bins per channel
 Histogram weight factors are    1.00000        0.00000
 No fixed background points for this powder pattern
 The  2 excluded regions are (in msec):
 Exclude    from:       to:     from:       to:     from:       to:     from:       to:
           0.0000    2.0000   20.0000 1000.0000
 Incident spectrum type  0 can be used in the region    1.000 msec to   20.000 msec
 The minimum possible weighted residual for this histogram is   0.0689
 Histogram no.  1 on file SAFE_NEUTRON_FINAL_STEPHANSS.P01
 updated with new excluded regions, background and incident spectrum data.
 CPU time =   0.01 to update histogram
 Lattice parameters for phase 1 are:
  a,b,c  =  5.202475  5.202475 14.014492  angles =    90.000    90.000   120.000
  volume =     328.494
 Lattice parameters for phase 2 are:
  a,b,c  =  5.202432  5.202446 14.014503  angles =    90.000    90.000   119.999
  volume =     328.494
 Profile function  3 for phase no. 1 has the coefficients p1-p21:
    0.289766E+00   0.528838E-01   0.746764E-02   0.000000E+00
    0.247120E+02   0.208014E+01   0.000000E+00   0.312672E+01
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00

    0.000000E+00
 cutoff on the wings at 0.001 of maximum

 Profile function  3 for phase no. 2 has the coefficients p1-p21:
    0.289766E+00   0.528838E-01   0.746764E-02   0.000000E+00
    0.247120E+02   0.208014E+01   0.000000E+00   0.312672E+01
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00

    0.000000E+00
 cutoff on the wings at 0.001 of maximum

 Minimum d-spacing used to generate reflections   0.4215 for phase 1
 Minimum d-spacing used to generate reflections   0.4215 for phase 2
 Minimum d-spacing used to generate reflections   0.9629 for phase 1
 Minimum d-spacing used to generate reflections   0.9629 for phase 2
 Minimum d-spacing for matching reflections   0.4370
 Estimated number of reflections to be generated is  1760
 Minimum d-spacing for magnetic reflections   1.0000
 Est. number of magnetic reflections to be generated is   914
 Number of reflections generated for phase 1 is   514
 Number of reflections generated for phase 2 is   794
 Total number of reflections generated for all phases is  1308
 CPU time =   0.01 sec. to generate reflections.
 CPU time =   0.13 sec. to locate reflection limits.
```

```
CPU time =   0.01 sec. to match reflection ranges to powder pattern
The maximum number of reflections contributing to any profile point is  204
CPU time =   0.01 sec. to update file
Data for bank  2 read from file c56881.gsa
The powder pattern has  3756 channels with   1 bins per channel
Histogram weight factors are    1.00000        0.00000
No fixed background points for this powder pattern
The  2 excluded regions are (in msec):
Exclude    from:       to:     from:       to:     from:       to:     from:       to:
          0.0000    2.9980   20.0000 1000.0000
Incident spectrum type  0 can be used in the region    1.000 msec to   20.000 msec
The number of zero intensities found in this histogram is    2
The minimum possible weighted residual for this histogram is   0.0391
Histogram no.  2 on file SAFE_NEUTRON_FINAL_STEPHANSS.P02
updated with new excluded regions, background and incident spectrum data.
CPU time =   0.01 to update histogram
Profile function  3 for phase no. 1 has the coefficients p1-p21:
   0.410819E+01   0.678940E-01   0.285702E-02   0.354299E+01
   0.439443E+02  -0.185852E+01   0.000000E+00   0.170472E-01
   0.162805E+01   0.000000E+00   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00

   0.000000E+00
cutoff on the wings at 0.001 of maximum

Profile function  3 for phase no. 2 has the coefficients p1-p21:
   0.410819E+01   0.678940E-01   0.285702E-02   0.354299E+01
   0.439443E+02  -0.185852E+01   0.000000E+00   0.170472E-01
   0.162805E+01   0.000000E+00   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00

   0.000000E+00
cutoff on the wings at 0.001 of maximum

Minimum d-spacing used to generate reflections   0.4738 for phase 1
Minimum d-spacing used to generate reflections   0.4738 for phase 2
Minimum d-spacing used to generate reflections   0.9765 for phase 1
Minimum d-spacing used to generate reflections   0.9765 for phase 2
Minimum d-spacing for matching reflections   0.4858
Estimated number of reflections to be generated is  1515
Minimum d-spacing for magnetic reflections   1.0000
Est. number of magnetic reflections to be generated is   878
Number of reflections generated for phase 1 is   359
Number of reflections generated for phase 2 is   734
Total number of reflections generated for all phases is  1093
CPU time =   0.01 sec. to generate reflections.
CPU time =   0.08 sec. to locate reflection limits.
CPU time =   0.01 sec. to match reflection ranges to powder pattern
The maximum number of reflections contributing to any profile point is  106
CPU time =   0.00 sec. to update file
Data for bank  3 read from file a56881.gsa
The powder pattern has  4821 channels with   1 bins per channel
Histogram weight factors are    1.00000        0.00000
No fixed background points for this powder pattern
The  2 excluded regions are (in msec):
Exclude    from:       to:     from:       to:     from:       to:     from:       to:
          0.0000    1.5520   20.0000 1000.0000
Incident spectrum type  0 can be used in the region    0.500 msec to   20.000 msec
The number of zero intensities found in this histogram is   13
The minimum possible weighted residual for this histogram is   0.1351
Histogram no.  3 on file SAFE_NEUTRON_FINAL_STEPHANSS.P03
updated with new excluded regions, background and incident spectrum data.
CPU time =   0.01 to update histogram
Profile function  3 for phase no. 1 has the coefficients p1-p21:
   0.100000E+01   0.527857E-01   0.202603E+00   0.219247E+02
   0.786456E+02   0.128369E+01   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00

   0.000000E+00
cutoff on the wings at 0.001 of maximum

Profile function  3 for phase no. 2 has the coefficients p1-p21:
```

```
   0.100000E+01   0.527857E-01   0.202603E+00   0.219247E+02
   0.786456E+02   0.128369E+01   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00

   0.000000E+00
 cutoff on the wings at 0.001 of maximum

 Minimum d-spacing used to generate reflections   0.7029 for phase 1
 Minimum d-spacing used to generate reflections   0.7029 for phase 2
 Minimum d-spacing used to generate reflections   0.9742 for phase 1
 Minimum d-spacing used to generate reflections   0.9742 for phase 2
 Minimum d-spacing for matching reflections   0.7206
 Estimated number of reflections to be generated is  1169
 Minimum d-spacing for magnetic reflections   1.0000
 Est. number of magnetic reflections to be generated is   884
 Number of reflections generated for phase 1 is   112
 Number of reflections generated for phase 2 is   746
 Total number of reflections generated for all phases is   858
 CPU time =   0.00 sec. to generate reflections.
 CPU time =   0.07 sec. to locate reflection limits.
 CPU time =   0.01 sec. to match reflection ranges to powder pattern
 The maximum number of reflections contributing to any profile point is  128
 CPU time =   0.01 sec. to update file
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             |-----------------------------------------------------|
             |            Program GENLES Version MacOSX            |
             |    General crystal structure refinement program     |
             | Magnetic structure refinement added by M. Yethiraj  |
             |   Revised and corrected by Larson and Von Dreele    |
             |      Distributed on Wed Apr 21 18:37:09 2010        |
             |-----------------------------------------------------|

        |-------------------------------------------------------------|
        |            Allen C. Larson and Robert B. Von Dreele         |
        |      Manuel Lujan, Jr. Neutron Scattering Center, MS-H805    |
        |      Los Alamos National Laboratory, Los Alamos, NM  87545  |
        |                                                             |
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        |-------------------------------------------------------------|

 The experiment file is: SAFE_NEUTRON_FINAL_STEPHANSS.EXP
 The last history record is :
     HSTRY 84 POWPREF MacOSX Jun 14 18:25:39 2011
 Maximum number of cycles is   99
 Marquardt factor for matrix inversion =  3.28
 I/SigI cut-off is  1.00
 Structure factors will be extracted from histogram  1
 using extraction method codes     0    0    0    0    0    0    0    0    0
 Structure factors will be extracted from histogram  2
 using extraction method codes     0    0    0    0    0    0    0    0    0
 Structure factors will be extracted from histogram  3
 using extraction method codes     0    0    0    0    0    0    0    0    0

 The atomic and magnetic scattering factors for  3 types of atoms are:
 Atom type   b-len     a(1)      b(1)      a(2)      b(2)      a(3)      b(3)      a(4)      b(4)      c
g
 SC+3        1.229   13.4008    0.2985    8.0273    7.9629    1.6594   -0.2860    1.5794   16.0662   -6.6667
 <j0> Mag. ff   :     0.5048   31.4040    0.5186   10.9900   -0.0241    1.1830    0.0000    0.0000    0.0000
 <j2> Mag. ff   :     4.3683   28.6540    3.7231   10.8230    0.6074    3.6680    0.0000    0.0000    0.0014
2.000
 FE+3        0.945   11.1764    4.6147    7.3863    0.3005    3.3948   11.6729    0.0724   38.5566    0.9707
 <j0> Mag. ff   :     0.3972   13.2440    0.6295    4.9030   -0.0314    0.3500    0.0000    0.0000    0.0044
 <j2> Mag. ff   :     1.3602   11.9980    1.5188    5.0030    0.4705    1.9910    0.0000    0.0000    0.0038
2.000
 O           0.580    3.0485   13.2771    2.2868    5.7011    1.5463    0.3239    0.8670   32.9089    0.2508
 Atom type      CrKa     FeKa     CuKa     MoKa     AgKa     TiKa     CoKa     TaKa      WKa      AuKa
 SC+3     f'   -0.694   -0.012    0.312    0.252    0.183   -5.426    0.147    0.016    0.013    0.002
          f"    2.965    2.256    1.533    0.372    0.235    4.002    1.977    0.034    0.032    0.023
 FE+3     f'   -1.294   -2.055   -1.134    0.346    0.289   -0.890   -3.331    0.044    0.039    0.017
          f"    0.762    0.565    3.197    0.844    0.545    1.052    0.490    0.084    0.079    0.058
 O        f'    0.093    0.072    0.049    0.011    0.006    0.121    0.063   -0.002   -0.003   -0.003
```

```
          f"    0.073    0.052    0.032    0.006    0.004    0.106    0.044    0.000    0.000    0.000
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 Space group  R 3 c
 The lattice is acentric  R-centered trigonal      Laue symmetry 3barm1
  Multiplicity of a general site is  18
  The location of the origin is arbitrary in z

 The equivalent positions are:

 ( 1)     X      Y      Z  ( 2)    -Y     X-Y     Z  ( 3)    Y-X    -X      Z
 ( 4)    Y-X     Y  1/2+Z  ( 5)    -Y     -X  1/2+Z  ( 6)     X     X-Y 1/2+Z


 The atom positions read in are: (all variable numbers (pn) are in hexadecimal)

 Type seq. At. name  mult   symm  frac   pn    X    pn    Y    pn    Z    pn  u11 pn  u22 pn  u33 pn  u12 pn  u13
pn  u23 pn
 SC+3    1 Sc1         6    3    0.4600   0 0.0000   0 0.0000   0 0.0477   1 0.4   2
 FE+3    2 Fe1         6    3    0.4600   0 0.0000   0 0.0000   0 0.2579   0 0.5   3
 O       3 O1         18    1    1.0000   0 0.3424   4-0.0260   5 0.8176   6 0.5   7
 FE+3    4 Fe2         6    3    0.5400   0 0.0000   0 0.0000   0 0.0477   8 0.4   9
 SC+3    5 Sc2         6    3    0.5400   0 0.0000   0 0.0000   0 0.2579   0 0.5   A

 Space group  P 1
 The lattice is acentric   primitive triclinic     Laue symmetry 1bar
  Multiplicity of a general site is   1
  The location of the origin is arbitrary in xyz

 The equivalent positions are:

 ( 1)     X      Y      Z

 Parameters to be held - 2  1MY   2  1MZ   2  2MY   2  2MZ   2  3MY   2  3MZ   2  4MY   2  4MZ
 Parameters to be held - 2  5MY   2  6MZ   2  7MZ   2  5MZ   2  6MY   2  7MY   2  8MY   2  8MZ
 Parameters to be held - 2  9MY   2  9MZ   2 10MY   2 10MZ   2 11MY   2 11MZ   2 12MZ   2 12MY
 Parameters to be held - 2  7X    2  7Y    2  8X    2  8Y    2  9X    2  9Y    2 10X    2 10Y
 Parameters to be held - 2 11X    2 11Y    2 12X    2 12Y

 All of the following data refer to the current space group symbol
 No antisymmetry operations are allowed

 The atom positions read in are: (all variable numbers (pn) are in hexadecimal)

 Type seq. At. name  mult   symm  frac   pn    X    pn    Y    pn    Z    pn  u11 pn  u22 pn  u33 pn  u12 pn  u13
pn  u23 pn
                                           Mx    pn   My    pn   Mz    pn
 FE+3    1 FE1         1    1    0.4600   0 0.0000   0 0.0000   0 0.2579   0 0.5   B
                                           2.672  C   0.000  0   0.000  0
 FE+3    2 FE2         1    1    0.4600   0 0.6667   0 0.3333   0 0.5912   0 0.5   D
                                           2.672  E   0.000  0   0.000  0
 FE+3    3 FE3         1    1    0.4600   0 0.3333   0 0.6667   0 0.9246   0 0.5   F
                                           2.672 10   0.000  0   0.000  0
 FE+3    4 FE4         1    1    0.4600   0 0.0000   0 0.0000   0 0.7579   0 0.5  11
                                          -2.672 12   0.000  0   0.000  0
 FE+3    5 FE5         1    1    0.4600   0 0.6667   0 0.3333   0 0.0912   0 0.5  13
                                          -2.672 14   0.000  0   0.000  0
 FE+3    6 FE6         1    1    0.4600   0 0.3333   0 0.6667   0 0.4246   0 0.5  15
                                          -2.672 16   0.000  0   0.000  0
 FE+3    7 FE7         1    1    0.5400   0 0.0000   0 0.0000   0 0.0477  17 0.4  18
                                          -2.672 19   0.000  0   0.000  0
 FE+3    8 FE8         1    1    0.5400   0 0.6667   0 0.3333   0 0.3810  1A 0.4  1B
                                          -2.672 1C   0.000  0   0.000  0
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 The atom positions read in are: (all variable numbers (pn) are in hexadecimal)

 Type seq. At. name  mult   symm  frac   pn    X    pn    Y    pn    Z    pn  u11 pn  u22 pn  u33 pn  u12 pn  u13
pn  u23 pn
                                           Mx    pn   My    pn   Mz    pn
 FE+3    9 FE9         1    1    0.5400   0 0.3333   0 0.6667   0 0.7144  1D 0.4  1E
                                          -2.672 1F   0.000  0   0.000  0
```

```
 FE+3   10 FE10        1    1    0.5400   0 0.0000   0 0.0000   0 0.5477  20 0.4  21
                                      2.672 22   0.000  0   0.000  0
 FE+3   11 FE11        1    1    0.5400   0 0.6667   0 0.3333   0 0.8810  23 0.4  24
                                      2.672 25   0.000  0   0.000  0
 FE+3   12 FE12        1    1    0.5400   0 0.3333   0 0.6667   0 0.2144  26 0.4  27
                                      2.672 28   0.000  0   0.000  0
  Constraints read are LNCN   1 1  1Z     1.0000 1  4Z     1.0000 2  7Z     1.0000 2  8Z     1.0000
                       LNCN   1 2  9Z     1.0000 2 10Z     1.0000 2 11Z     1.0000 2 12Z     1.0000
                       LNCN   2 1  1FRAC -1.0000 1  2FRAC -1.0000 1  4FRAC  1.0000 1  5FRAC  1.0000
 Parameter missing - 1  1FRAC
 Parameter missing - 1  2FRAC
 Parameter missing - 1  4FRAC
 Parameter missing - 1  5FRAC
                       LNCN   2 2  1FRAC -1.0000 2  2FRAC -1.0000 2  3FRAC -1.0000 2  4FRAC -1.0000
 Parameter missing - 2  1FRAC
 Parameter missing - 2  2FRAC
 Parameter missing - 2  3FRAC
 Parameter missing - 2  4FRAC
                       LNCN   2 2  5FRAC -1.0000 2  6FRAC -1.0000 2  7FRAC  1.0000 2  8FRAC  1.0000
 Parameter missing - 2  5FRAC
 Parameter missing - 2  6FRAC
 Parameter missing - 2  7FRAC
 Parameter missing - 2  8FRAC
                       LNCN   2 2  9FRAC  1.0000 2 10FRAC  1.0000 2 11FRAC  1.0000 2 12FRAC  1.0000
 Parameter missing - 2  9FRAC
 Parameter missing - 2 10FRAC
 Parameter missing - 2 11FRAC
 Parameter missing - 2 12FRAC
                       LNCN   3 1  2Z     1.0000 1  5Z     1.0000 2  1Z     1.0000 2  2Z     1.0000
 Parameter missing - 1  2Z
 Parameter missing - 1  5Z
 Parameter missing - 2  1Z
 Parameter missing - 2  2Z
                       LNCN   3 2  3Z     1.0000 2  4Z     1.0000 2  5Z     1.0000 2  6Z     1.0000
 Parameter missing - 2  3Z
 Parameter missing - 2  4Z
 Parameter missing - 2  5Z
 Parameter missing - 2  6Z
                       LNCN   4 1  1UISO  1.0000 1  4UISO  1.0000 2  7UISO  1.0000 2  8UISO  1.0000
                       LNCN   4 2  9UISO  1.0000 2 10UISO  1.0000 2 11UISO  1.0000 2 12UISO  1.0000
                       LNCN   5 2  1MX    1.0000 2  2MX    1.0000 2  3MX    1.0000 2 10MX    1.0000
                       LNCN   5 2 11MX    1.0000 2 12MX    1.0000 2  4MX   -1.0000 2  5MX   -1.0000
                       LNCN   5 2  6MX   -1.0000 2  7MX   -1.0000 2  8MX   -1.0000 2  9MX   -1.0000
                       LNCN   6 1  2UISO  1.0000 1  5UISO  1.0000 2  1UISO  1.0000 2  2UISO  1.0000
                       LNCN   6 2  3UISO  1.0000 2  4UISO  1.0000 2  5UISO  1.0000 2  6UISO  1.0000
 Constraint no.  1 for type RMTN:   1    RM33     1.0000 2    RM33     1.0000
 Constraint no.  2 for type RMTN:   1    RM11     1.0000 2    RM11     1.0000 2    RM22     1.0000
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 Lattice parameters for phase 1 are:
     a          b          c          alpha      beta     gamma
    5.202475   5.202475  14.014492   90.0000   90.0000  120.0000
 These cell parameters will be refined
 Reciprocal metric tensor elements:          damp= 0
 Element :          g11   pn          g22   pn          g33   pn        2*g12   pn        2*g13   pn        2*g23
pn
 Value   :   4.92628E-02  29   4.92628E-02  2A   5.09149E-03  2B   4.92628E-02  2C  -6.67560E-10   0
-6.67560E-10   0
 Constr. :          1.000  2          1.000  2          1.000  2          1.000  2          0.000  0
0.000  0

 Lattice parameters for phase 2 are:
     a          b          c          alpha      beta     gamma
    5.202432   5.202446  14.014503   90.0000   90.0000  119.9987
 These cell parameters will be refined
 Reciprocal metric tensor elements:          damp= 0
 Element :          g11   pn          g22   pn          g33   pn        2*g12   pn        2*g13   pn        2*g23
pn
 Value   :   4.92623E-02  2D   4.92620E-02  2E   5.09149E-03  2F   4.92602E-02   0  -6.67539E-10   0
-6.67537E-10   0
 Constr. :          1.000  2          1.000  2          1.000  2          1.000  0          1.000  0
1.000  0

 Phase/element fractions for phase no.  1
```

```
 Hist Elm:    PNT   1 1   nc    PNT   2 1   nc    PNT   3 1   nc    PNT*  4 1   nc    PXC*  5 1   nc
 Fraction:    1.0000       0    1.0000       0    1.0000       0   not present       not present
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0

 Phase/element fractions for phase no.  2

 Hist Elm:    PNT   1 1   nc    PNT   2 1   nc    PNT   3 1   nc    PNT*  4 1   nc    PXC*  5 1   nc
 Fraction:    1.0000       0    1.0000       0    1.0000       0   not present       not present
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0

 Histogram scale factors:

 Hist/Typ:    1  PNT      pn    2  PNT      pn    3  PNT      pn    4  PNT*     pn    5  PXC*     pn
 Scale   :    8.7594      30    8.7618      31    10.066      32    0.0000       0    0.0000       0
 Dmp/Cnst:    0     1.000  3    0     1.000  4    0     1.000  5    0     0.000  0    0     0.000  0

 Absorption coefficients for powder data:

 Hist/Typ:    1  PNT    0 pn    2  PNT    0 pn    3  PNT    0 pn    4  PNT*   0 pn    5  PXC*   0 pn
 Absc 1. :   0.21758E-01   0   0.21758E-01   0   0.21758E-01   0    0.0000       0    0.0000       0
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0
 Absc 2. :    0.0000       0    0.0000       0    0.0000       0    0.0000       0    0.0000       0
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0
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 Diffractometer constants for powder data:
 No. Type    Dif C   pn    Dif A   pn     Zero    pn Cnstr  cn Damp
  1  PNT    4569.20  33     -0.97  35     1.900    0 0.000   0    0
 No. Type    Dif C   pn    Dif A   pn     Zero    pn Cnstr  cn Damp
  2  PNT    6162.13   0     -2.51   0     3.850    0 0.000   0    0
 No. Type    Dif C   pn    Dif A   pn     Zero    pn Cnstr  cn Damp
  3  PNT    2139.59  34      1.30  36     9.030    0 0.000   0    0

 Extinction coefficients for phase no.  1:

 Hist/Typ:    1  PNT      pn    2  PNT      pn    3  PNT      pn    4  PNT*     pn    5  PXC*     pn
 Extinct.:    0.0000       0    0.0000       0    0.0000       0    0.0000       0    0.0000       0
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0

 Extinction coefficients for phase no.  2:

 Hist/Typ:    1  PNT      pn    2  PNT      pn    3  PNT      pn    4  PNT*     pn    5  PXC*     pn
 Extinct.:    0.0000       0    0.0000       0    0.0000       0    0.0000       0   not present
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0

 Radiation damage coefficients for phase no.  1:

 Hist/Typ:    1  PNT      pn    2  PNT      pn    3  PNT      pn    4  PNT*     pn    5  PXC*     pn
 Rad.dam.:    0.0000       0    0.0000       0    0.0000       0    0.0000       0    0.0000       0
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0

 Radiation damage coefficients for phase no.  2:

 Hist/Typ:    1  PNT      pn    2  PNT      pn    3  PNT      pn    4  PNT*     pn    5  PXC*     pn
 Rad.dam.:    0.0000       0    0.0000       0    0.0000       0    0.0000       0   not present
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0

 Preferred orientation coeffs. for phase no.  1 histogram no.  1:
 Axis    :        1       pn
 Dir./typ:    0.0 0.0 1.0  0
 PO ratio:        1.0000   0
 Dmp/Cnst:    0     0.000  0
 PO frac.:        1.0000   0
 Dmp/Cnst:    0     0.000  0
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 Preferred orientation coeffs. for phase no.  1 histogram no.  2:
 Axis    :        1       pn
 Dir./typ:    0.0 0.0 1.0  0
 PO ratio:        1.0000   0
 Dmp/Cnst:    0     0.000  0
```

```
 PO frac.:        1.0000   0
 Dmp/Cnst:    0     0.000  0

 Preferred orientation coeffs. for phase no.  1 histogram no.  3:
 Axis    :        1       pn
 Dir./typ:    0.0 0.0 1.0  0
 PO ratio:        1.0000   0
 Dmp/Cnst:    0     0.000  0
 PO frac.:        1.0000   0
 Dmp/Cnst:    0     0.000  0

 Preferred orientation coeffs. for phase no.  2 histogram no.  1:
 Axis    :        1       pn
 Dir./typ:    0.0 0.0 1.0  0
 PO ratio:        1.0000   0
 Dmp/Cnst:    0     0.000  0
 PO frac.:        1.0000   0
 Dmp/Cnst:    0     0.000  0

 Preferred orientation coeffs. for phase no.  2 histogram no.  2:
 Axis    :        1       pn
 Dir./typ:    0.0 0.0 1.0  0
 PO ratio:        1.0000   0
 Dmp/Cnst:    0     0.000  0
 PO frac.:        1.0000   0
 Dmp/Cnst:    0     0.000  0

 Preferred orientation coeffs. for phase no.  2 histogram no.  3:
 Axis    :        1       pn
 Dir./typ:    0.0 0.0 1.0  0
 PO ratio:        1.0000   0
 Dmp/Cnst:    0     0.000  0
 PO frac.:        1.0000   0
 Dmp/Cnst:    0     0.000  0


 Constraint no.  1 for type PF 5:   ALL,1         1.000
 Constraint no.  2 for type PF 5:   ALL,2         1.000
 Constraint no.  3 for type PF 5:   ALL,3         1.000

 Constraint no.  1 for type PF 8:   ALL,1         1.000
 Constraint no.  2 for type PF 8:   ALL,2         1.000
 Constraint no.  3 for type PF 8:   ALL,3         1.000
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 Profile coeff. for function type  3, phase no.  1 and histogram no.  1; aniso. axis   0.   0.   1.; damp= 0:
 Coeff.  :     alp    pn     be-0   pn     be-1   pn     sg-0   pn     sg-1   pn     sg-2   pn     ga-0   pn
ga-1   pn
 Value   : 2.898E-01   0 5.288E-02   0 7.468E-03   0 0.000E+00   0 2.471E+01  37 2.080E+00   0 0.000E+00   0
3.127E+00  3D
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      1.000 10      0.000  0      0.000  0
1.000 13
 Coeff.  :     ga-2   pn     gsf    pn     g1ec   pn     g2ec   pn     rstr   pn     rsta   pn     rsca   pn
L11    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
0.000  0
 Coeff.  :     L22    pn     L33    pn     L12    pn     L13    pn     L23    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0

 Profile coeff. for function type  3, phase no.  1 and histogram no.  2; aniso. axis   0.   0.   1.; damp= 0:
 Coeff.  :     alp    pn     be-0   pn     be-1   pn     sg-0   pn     sg-1   pn     sg-2   pn     ga-0   pn
ga-1   pn
 Value   : 4.108E+00   0 6.789E-02   0 2.857E-03   0 3.543E+00   0 4.394E+01  38-1.859E+00   0 0.000E+00   0
1.705E-02  3E
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      1.000 11      0.000  0      0.000  0
1.000 14
 Coeff.  :     ga-2   pn     gsf    pn     g1ec   pn     g2ec   pn     rstr   pn     rsta   pn     rsca   pn
L11    pn
 Value   : 1.628E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
```

```
0.000  0
 Coeff.  :     L22    pn     L33    pn     L12    pn     L13    pn     L23    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0

 Profile coeff. for function type  3, phase no.  1 and histogram no.  3; aniso. axis   0.   0.   1.; damp= 0:
 Coeff.  :     alp    pn     be-0   pn     be-1   pn     sg-0   pn     sg-1   pn     sg-2   pn     ga-0   pn
ga-1   pn
 Value   : 1.000E+00   0 5.279E-02   0 2.026E-01   0 2.192E+01   0 7.865E+01  39 1.284E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      1.000 12      0.000  0      0.000  0
0.000  0
 Coeff.  :     ga-2   pn     gsf    pn     g1ec   pn     g2ec   pn     rstr   pn     rsta   pn     rsca   pn
L11    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
0.000  0
 Coeff.  :     L22    pn     L33    pn     L12    pn     L13    pn     L23    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0

 Profile coeff. for function type  3, phase no.  2 and histogram no.  1; aniso. axis   0.   0.   1.; damp= 0:
 Coeff.  :     alp    pn     be-0   pn     be-1   pn     sg-0   pn     sg-1   pn     sg-2   pn     ga-0   pn
ga-1   pn
 Value   : 2.898E-01   0 5.288E-02   0 7.468E-03   0 0.000E+00   0 2.471E+01  3A 2.080E+00   0 0.000E+00   0
3.127E+00  3F
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      1.000 10      0.000  0      0.000  0
1.000 13
 Coeff.  :     ga-2   pn     gsf    pn     g1ec   pn     g2ec   pn     rstr   pn     rsta   pn     rsca   pn
L11    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
0.000  0
 Coeff.  :     L22    pn     L33    pn     L12    pn     L13    pn     L23    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0

 Profile coeff. for function type  3, phase no.  2 and histogram no.  2; aniso. axis   0.   0.   1.; damp= 0:
 Coeff.  :     alp    pn     be-0   pn     be-1   pn     sg-0   pn     sg-1   pn     sg-2   pn     ga-0   pn
ga-1   pn
 Value   : 4.108E+00   0 6.789E-02   0 2.857E-03   0 3.543E+00   0 4.394E+01  3B-1.859E+00   0 0.000E+00   0
1.705E-02  40
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      1.000 11      0.000  0      0.000  0
1.000 14
 Coeff.  :     ga-2   pn     gsf    pn     g1ec   pn     g2ec   pn     rstr   pn     rsta   pn     rsca   pn
L11    pn
 Value   : 1.628E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
0.000  0
 Coeff.  :     L22    pn     L33    pn     L12    pn     L13    pn     L23    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
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 Profile coeff. for function type  3, phase no.  2 and histogram no.  3; aniso. axis   0.   0.   1.; damp= 0:
 Coeff.  :     alp    pn     be-0   pn     be-1   pn     sg-0   pn     sg-1   pn     sg-2   pn     ga-0   pn
ga-1   pn
 Value   : 1.000E+00   0 5.279E-02   0 2.026E-01   0 2.192E+01   0 7.865E+01  3C 1.284E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      1.000 12      0.000  0      0.000  0
0.000  0
 Coeff.  :     ga-2   pn     gsf    pn     g1ec   pn     g2ec   pn     rstr   pn     rsta   pn     rsca   pn
L11    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
0.000  0
 Coeff.  :     L22    pn     L33    pn     L12    pn     L13    pn     L23    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
```

```
 Diffuse scattering coefficients for powder data:
 No diffuse scattering coefficients for histogram    1
 No diffuse scattering coefficients for histogram    2
 No diffuse scattering coefficients for histogram    3

 Background coefficients for powder data:
 Histogram no.:    1 Damping factor:    0 Use all points: Y
 Shifted Chebyshev function of first kind
 Param.  :          1   pn          2   pn          3   pn          4   pn          5   pn          6   pn
 Coeff.  : 0.33101E+00  41-0.16476E-01  43 0.53839E-01  45-0.17364E-01  47-0.89158E-02  49-0.38795E-01  4B
 Param.  :          7   pn          8   pn          9   pn
 Coeff.  :-0.17909E-01  4D-0.14925E-01  4F-0.69492E-02  51
 Histogram no.:    2 Damping factor:    0 Use all points: Y
 Shifted Chebyshev function of first kind
 Param.  :          1   pn          2   pn          3   pn          4   pn          5   pn          6   pn
 Coeff.  : 0.27396E+00  42-0.97415E-01  44 0.96659E-02  46-0.17507E-01  48 0.11207E-01  4A-0.81016E-02  4C
 Param.  :          7   pn          8   pn          9   pn         10   pn         11   pn         12   pn
 Coeff.  : 0.30981E-03  4E-0.14559E-01  50-0.64751E-02  52 0.24006E-02  53 0.39535E-02  54-0.16723E-01  55
 Histogram no.:    3 Damping factor:    0 Use all points: Y
 Shifted Chebyshev function of first kind
 Param.  :          1   pn          2   pn          3   pn          4   pn          5   pn          6   pn
 Coeff.  : 0.29912E+00   0-0.31899E-01   0-0.42900E-02   0-0.15951E-01   0 0.19462E-01   0-0.11893E-01   0
 Param.  :          7   pn          8   pn          9   pn         10   pn
 Coeff.  :-0.25533E-01   0 0.40060E-02   0 0.13208E-01   0-0.14414E-01   0

 The constraint matrix has     85 terms
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 Restraint data statistics:
 No restraints used

 Powder data statistics                Fitted         -Bknd          pFree                  Average
              Bank Ndata Sum(w*d**2)  wRp     Rp    wRp     Rp    wRp     Rp  Npfree  DWd  Integral
 Hstgm  1 PNT   1  4524  4595.5     0.0694 0.1158 3.0671 0.6237 0.0000 0.0000     0   0.658   0.982
 Hstgm  2 PNT   2  3753  4939.7     0.0449 0.0942 0.1097 0.1130 0.0000 0.0000     0   0.462   0.990
 Hstgm  3 PNT   3  4808  4302.5     0.1278 0.1742 3.2083 0.7146 0.0000 0.0000     0   0.733   0.997
 Powder totals    13085  13838.     0.0614 0.1235 1.9261 0.4498 0.0000 0.0000     0   0.611

 No serial correlation in fit at 90% confidence for 1.952 < DWd < 2.048
 Cycle1155 There were  13085 observations.
 Total before-cycle CHI**2 (offset/sig) = 1.3838E+04 ( 4.9271E+00)
 Reduced CHI**2 =  1.061     for   43 variables

 Reflection data statistics
 Histogram  1  Type PNT   Nobs = 1302 R(F**2) =  0.1131
 Histogram  2  Type PNT   Nobs = 1071 R(F**2) =  0.0970
 Histogram  3  Type PNT   Nobs =  857 R(F**2) =  0.0802
 Marquardt factor for this cycle =   3.28
 After matrix normalization and Marquardt modification:

    1 Columns of the    43 Column matrix are 0.0
 Full matrix recip. condition value & -log10 =   0.1169          0.93
         Variable NoVarabl was not refined

 The value of the determinant is  1.0307*10.0**(    -1)

 Atom parameters for phase no. 1
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
 SC+3  (  1) Values  : 0.460  0.000000  0.000000  0.047687    0.378
             Sigmas  :                             0.000048    0.005
             Shft/esd:                               -0.01    -0.01
 Sc1      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  2) Values  : 0.460  0.000000  0.000000  0.257903    0.510
             Sigmas  :                                       0.005
             Shft/esd:                                        0.04
 Fe1      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 O     (  3) Values  : 1.000  0.342431 -0.026015  0.817575    0.481
             Sigmas  :        0.000153  0.000095  0.000209    0.005
             Shft/esd:           -0.01     -0.03      0.00     0.03
 O1       moved  0.00A     sum(shift/e.s.d)**2 :    0.00
```

```
 FE+3  (  4) Values  : 0.540  0.000000  0.000000  0.047687    0.378
            Sigmas  :                             0.000048    0.005
            Shft/esd:                               -0.01    -0.01
 Fe2      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

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 SC+3  (  5) Values  : 0.540  0.000000  0.000000  0.257903    0.510
            Sigmas  :                                       0.005
            Shft/esd:                                        0.04
 Sc2      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 1 :      0.01
 Calculated unit cell formula weight:   892.800, density:  4.513gm/cm**3

 Atom parameters for phase no. 2
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
                               Mx        My        Mz     |Moment|   Theta    Psi
 FE+3  (  1) Values  : 0.460  0.000000  0.000000  0.257890    0.510
            Sigmas  :                                       0.005
            Shft/esd:                                        0.04

 FE+3  (  1) Moments :           2.672     0.000     0.000    2.672   90.000    0.000
            Sigmas  :           0.042                         0.042    0.000    0.000
            Shft/esd:            0.00
 FE1      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  2) Values  : 0.460  0.666670  0.333330  0.591220    0.510
            Sigmas  :                                       0.005
            Shft/esd:                                        0.04

 FE+3  (  2) Moments :           2.672     0.000     0.000    2.672   90.000    0.000
            Sigmas  :           0.042                         0.042    0.000    0.000
            Shft/esd:            0.00
 FE2      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  3) Values  : 0.460  0.333330  0.666670  0.924560    0.510
            Sigmas  :                                       0.005
            Shft/esd:                                        0.04

 FE+3  (  3) Moments :           2.672     0.000     0.000    2.672   90.000    0.000
            Sigmas  :           0.042                         0.042    0.000    0.000
            Shft/esd:            0.00
 FE3      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  4) Values  : 0.460  0.000000  0.000000  0.757890    0.510
            Sigmas  :                                       0.005
            Shft/esd:                                        0.04

 FE+3  (  4) Moments :          -2.672     0.000     0.000    2.672   90.000  180.000
            Sigmas  :           0.042                         0.042    0.000    0.000
            Shft/esd:            0.00
 FE4      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

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 FE+3  (  5) Values  : 0.460  0.666670  0.333330  0.091220    0.510
            Sigmas  :                                       0.005
            Shft/esd:                                        0.04

 FE+3  (  5) Moments :          -2.672     0.000     0.000    2.672   90.000  180.000
            Sigmas  :           0.042                         0.042    0.000    0.000
            Shft/esd:            0.00
 FE5      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  6) Values  : 0.460  0.333330  0.666670  0.424560    0.510
            Sigmas  :                                       0.005
            Shft/esd:                                        0.04

 FE+3  (  6) Moments :          -2.672     0.000     0.000    2.672   90.000  180.000
            Sigmas  :           0.042                         0.042    0.000    0.000
            Shft/esd:            0.00
```

```
 FE6      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  7) Values  : 0.540  0.000000  0.000000  0.047687    0.378
             Sigmas  :                             0.000048    0.005
             Shft/esd:                                -0.01    -0.01

 FE+3  (  7) Moments :          -2.672     0.000     0.000    2.672   90.000  180.000
             Sigmas  :           0.042                         0.042    0.000    0.000
             Shft/esd:            0.00
 FE7      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  8) Values  : 0.540  0.666670  0.333330  0.381017    0.378
             Sigmas  :                             0.000048    0.005
             Shft/esd:                                -0.01    -0.01

 FE+3  (  8) Moments :          -2.672     0.000     0.000    2.672   90.000  180.000
             Sigmas  :           0.042                         0.042    0.000    0.000
             Shft/esd:            0.00
 FE8      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  9) Values  : 0.540  0.333330  0.666670  0.714358    0.378
             Sigmas  :                             0.000048    0.005
             Shft/esd:                                -0.01    -0.01

 FE+3  (  9) Moments :          -2.672     0.000     0.000    2.672   90.000  180.000
             Sigmas  :           0.042                         0.042    0.000    0.000
             Shft/esd:            0.00
 FE9      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

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 FE+3  ( 10) Values  : 0.540  0.000000  0.000000  0.547688    0.378
             Sigmas  :                             0.000048    0.005
             Shft/esd:                                -0.01    -0.01

 FE+3  ( 10) Moments :           2.672     0.000     0.000    2.672   90.000    0.000
             Sigmas  :           0.042                         0.042    0.000    0.000
             Shft/esd:            0.00
 FE10     moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  ( 11) Values  : 0.540  0.666670  0.333330  0.881018    0.378
             Sigmas  :                             0.000048    0.005
             Shft/esd:                                -0.01    -0.01

 FE+3  ( 11) Moments :           2.672     0.000     0.000    2.672   90.000    0.000
             Sigmas  :           0.042                         0.042    0.000    0.000
             Shft/esd:            0.00
 FE11     moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  ( 12) Values  : 0.540  0.333330  0.666670  0.214358    0.378
             Sigmas  :                             0.000048    0.005
             Shft/esd:                                -0.01    -0.01

 FE+3  ( 12) Moments :           2.672     0.000     0.000    2.672   90.000    0.000
             Sigmas  :           0.042                         0.042    0.000    0.000
             Shft/esd:            0.00
 FE12     moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 2 :      0.01
 Calculated unit cell formula weight:   335.082, density:  1.694gm/cm**3

 Histogram scale factors:

 Histogram:    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 Scale    :    8.75995        8.76258        10.0662        0.00000        0.00000
 Sigmas   :   0.195795E-01   0.133013E-01   0.343965E-01    0.00000        0.00000
 Shift/esd:       0.03           0.06           0.01           0.00           0.00
 Histogram scale factor sum(shift/error)**2 :      0.00

 Lattice parameters for powder data:
 Phase  1
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202475  5.202475 14.014490    90.000    90.000   120.000     328.494
 Sigmas   :  0.000004  0.000004  0.000104     0.000     0.000     0.000       0.003
```

```
 Recprocal metric tensor shift factor = 100%
 Phase  2
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202432  5.202446 14.014501    90.000    90.000   119.999     328.494
 Sigmas   :  0.000007  0.000007  0.000104     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Recprocal metric tensor sum(shift/error)**2 :      0.00
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 Diffractometer coefficients for powder data:
 Histogram :    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 C/L1/R/2Th:    4569.20        6162.13        2139.59        0.00000        0.00000
 Sigmas    :   0.354186E-01    0.00000       0.493411E-01    0.00000        0.00000
 Shift/esd :      -0.01           0.00          -0.03           0.00           0.00
 Dif A/Pola:  -0.970326       -2.51000        1.29919        0.00000        0.00000
 Sigmas    :   0.222295E-01    0.00000       0.224544E-01    0.00000        0.00000
 Shift/esd :      -0.01           0.00          -0.03           0.00           0.00
 Zero      :    1.90000        3.85000        9.03000        0.00000        0.00000
 Sigmas    :    0.00000        0.00000        0.00000        0.00000        0.00000
 Shift/esd :      -0.01           0.00          -0.03           0.00           0.00
 Dif. Cons. Sum(shift/error)**2 :      0.00

 Profile coefficients for histogram no.  1 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.471E+01  2.080E+00  0.000E+00  3.128E+00  0.000E+00
0.000E+00
 Sigmas   :                                              4.847E-01                        7.620E-02
 Shift/esd:                                                 -0.01                             0.01
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.394E+01 -1.859E+00  0.000E+00  1.798E-02  1.628E+00
0.000E+00
 Sigmas   :                                              3.832E-01                        4.968E-02
 Shift/esd:                                                 -0.01                             0.02
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.318E-01
 Shift/esd:                                                 0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
```

```
 Shift/esd:
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 Profile coefficients for histogram no.  1 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.471E+01  2.080E+00  0.000E+00  3.128E+00  0.000E+00
0.000E+00
 Sigmas   :                                             4.847E-01                        7.620E-02
 Shift/esd:                                                -0.01                             0.01
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.394E+01 -1.859E+00  0.000E+00  1.798E-02  1.628E+00
0.000E+00
 Sigmas   :                                             3.832E-01                        4.968E-02
 Shift/esd:                                                -0.01                             0.02
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                             8.318E-01
 Shift/esd:                                                0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
 Profile coef. sum(shift/error)**2 :      0.00

 Background coefficients for histogram no.  1:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   3.310211E-01  -1.648528E-02   5.383977E-02  -1.736754E-02  -8.912571E-03  -3.879977E-02
 Sigmas   :   6.026234E-04   8.385003E-04   1.042685E-03   8.941636E-04   8.445025E-04   8.442385E-04
 Shift/esd:           0.01          -0.01           0.00           0.00           0.00          -0.01
 Param.   :           7             8             9
 Coeff.   :  -1.790531E-02  -1.492775E-02  -6.956429E-03
 Sigmas   :   8.422572E-04   8.461432E-04   8.279863E-04
 Shift/esd:           0.00           0.00          -0.01
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 Background coefficients for histogram no.  2:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   2.739718E-01  -9.743177E-02   9.673394E-03  -1.750218E-02   1.120425E-02  -8.098410E-03
```

```
 Sigmas   :   3.743019E-04   4.858084E-04   6.158429E-04   5.772837E-04   5.432102E-04   5.315255E-04
 Shift/esd:           0.03          -0.03           0.01           0.01           0.00           0.01
 Param.   :              7              8              9             10             11             12
 Coeff.   :   3.132125E-04  -1.456232E-02  -6.476350E-03   2.397511E-03   3.950211E-03  -1.672466E-02
 Sigmas   :   5.307376E-04   5.276806E-04   5.248352E-04   5.165430E-04   5.124614E-04   5.124906E-04
 Shift/esd:           0.01          -0.01           0.00          -0.01          -0.01           0.00
 Background coef. sum(shift/error)**2 :      0.00

 CPU times for matrix build     1.52 sec; matrix inversion     0.01 sec
 Final variable sum((shift/esd)**2) for cycle1155:       0.01 Time:    1.52 sec
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 Restraint data statistics:
 No restraints used

 Powder data statistics                Fitted         -Bknd          pFree                  Average
              Bank Ndata Sum(w*d**2)  wRp     Rp    wRp     Rp    wRp     Rp  Npfree  DWd  Integral
 Hstgm  1 PNT   1  4524  4595.4     0.0694 0.1158 3.0672 0.6237 0.0000 0.0000     0   0.658   0.982
 Hstgm  2 PNT   2  3753  4939.6     0.0449 0.0942 0.1097 0.1131 0.0000 0.0000     0   0.462   0.990
 Hstgm  3 PNT   3  4808  4302.6     0.1278 0.1742 3.2083 0.7146 0.0000 0.0000     0   0.733   0.997
 Powder totals    13085  13838.     0.0614 0.1235 1.9262 0.4499 0.0000 0.0000     0   0.611

 No serial correlation in fit at 90% confidence for 1.952 < DWd < 2.048
 Cycle1156 There were  13085 observations.
 Total before-cycle CHI**2 (offset/sig) = 1.3838E+04 ( 4.9259E+00)
 Reduced CHI**2 =  1.061     for   43 variables

 Reflection data statistics
 Histogram  1  Type PNT   Nobs = 1302 R(F**2) =  0.1131
 Histogram  2  Type PNT   Nobs = 1071 R(F**2) =  0.0970
 Histogram  3  Type PNT   Nobs =  857 R(F**2) =  0.0805
 Marquardt factor for this cycle =   3.28
 After matrix normalization and Marquardt modification:

    1 Columns of the    43 Column matrix are 0.0
 Full matrix recip. condition value & -log10 =   0.1169          0.93
        Variable NoVarabl was not refined

 The value of the determinant is  1.0306*10.0**(    -1)

 Atom parameters for phase no. 1
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
 SC+3  (  1) Values  : 0.460  0.000000  0.000000  0.047686    0.378
             Sigmas  :                             0.000048    0.005
             Shft/esd:                                0.00    -0.01
 Sc1      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  2) Values  : 0.460  0.000000  0.000000  0.257903    0.510
             Sigmas  :                                       0.005
             Shft/esd:                                        0.04
 Fe1      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 O     (  3) Values  : 1.000  0.342428 -0.026017  0.817575    0.482
             Sigmas  :        0.000153  0.000095  0.000209    0.005
             Shft/esd:           -0.02     -0.02      0.00     0.03
 O1       moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  4) Values  : 0.540  0.000000  0.000000  0.047686    0.378
             Sigmas  :                             0.000048    0.005
             Shft/esd:                                0.00    -0.01
 Fe2      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

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 SC+3  (  5) Values  : 0.540  0.000000  0.000000  0.257903    0.510
             Sigmas  :                                       0.005
             Shft/esd:                                        0.04
 Sc2      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 1 :      0.01
 Calculated unit cell formula weight:   892.800, density:  4.513gm/cm**3
```

```
 Atom parameters for phase no. 2
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
                                Mx        My        Mz     |Moment|   Theta    Psi
 FE+3  (  1) Values  : 0.460  0.000000  0.000000  0.257890    0.510
             Sigmas  :                                      0.005
             Shft/esd:                                       0.04

 FE+3  (  1) Moments :           2.672     0.000     0.000    2.672   90.000    0.000
             Sigmas  :           0.042                        0.042    0.000    0.000
             Shft/esd:            0.00
 FE1      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  2) Values  : 0.460  0.666670  0.333330  0.591220    0.510
             Sigmas  :                                      0.005
             Shft/esd:                                       0.04

 FE+3  (  2) Moments :           2.672     0.000     0.000    2.672   90.000    0.000
             Sigmas  :           0.042                        0.042    0.000    0.000
             Shft/esd:            0.00
 FE2      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  3) Values  : 0.460  0.333330  0.666670  0.924560    0.510
             Sigmas  :                                      0.005
             Shft/esd:                                       0.04

 FE+3  (  3) Moments :           2.672     0.000     0.000    2.672   90.000    0.000
             Sigmas  :           0.042                        0.042    0.000    0.000
             Shft/esd:            0.00
 FE3      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  4) Values  : 0.460  0.000000  0.000000  0.757890    0.510
             Sigmas  :                                      0.005
             Shft/esd:                                       0.04

 FE+3  (  4) Moments :          -2.672     0.000     0.000    2.672   90.000  180.000
             Sigmas  :           0.042                        0.042    0.000    0.000
             Shft/esd:            0.00
 FE4      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

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 FE+3  (  5) Values  : 0.460  0.666670  0.333330  0.091220    0.510
             Sigmas  :                                      0.005
             Shft/esd:                                       0.04

 FE+3  (  5) Moments :          -2.672     0.000     0.000    2.672   90.000  180.000
             Sigmas  :           0.042                        0.042    0.000    0.000
             Shft/esd:            0.00
 FE5      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  6) Values  : 0.460  0.333330  0.666670  0.424560    0.510
             Sigmas  :                                      0.005
             Shft/esd:                                       0.04

 FE+3  (  6) Moments :          -2.672     0.000     0.000    2.672   90.000  180.000
             Sigmas  :           0.042                        0.042    0.000    0.000
             Shft/esd:            0.00
 FE6      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  7) Values  : 0.540  0.000000  0.000000  0.047686    0.378
             Sigmas  :                            0.000048    0.005
             Shft/esd:                               0.00    -0.01

 FE+3  (  7) Moments :          -2.672     0.000     0.000    2.672   90.000  180.000
             Sigmas  :           0.042                        0.042    0.000    0.000
             Shft/esd:            0.00
 FE7      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  8) Values  : 0.540  0.666670  0.333330  0.381016    0.378
             Sigmas  :                            0.000048    0.005
             Shft/esd:                               0.00    -0.01

 FE+3  (  8) Moments :          -2.672     0.000     0.000    2.672   90.000  180.000
```

```
            Sigmas  :           0.042                        0.042    0.000    0.000
            Shft/esd:            0.00
 FE8      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  9) Values  : 0.540  0.333330  0.666670  0.714357    0.378
            Sigmas  :                             0.000048    0.005
            Shft/esd:                                0.00    -0.01

 FE+3  (  9) Moments :          -2.672     0.000     0.000    2.672   90.000  180.000
            Sigmas  :           0.042                        0.042    0.000    0.000
            Shft/esd:            0.00
 FE9      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

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 FE+3  ( 10) Values  : 0.540  0.000000  0.000000  0.547687    0.378
            Sigmas  :                             0.000048    0.005
            Shft/esd:                                0.00    -0.01

 FE+3  ( 10) Moments :           2.672     0.000     0.000    2.672   90.000    0.000
            Sigmas  :           0.042                        0.042    0.000    0.000
            Shft/esd:            0.00
 FE10     moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  ( 11) Values  : 0.540  0.666670  0.333330  0.881017    0.378
            Sigmas  :                             0.000048    0.005
            Shft/esd:                                0.00    -0.01

 FE+3  ( 11) Moments :           2.672     0.000     0.000    2.672   90.000    0.000
            Sigmas  :           0.042                        0.042    0.000    0.000
            Shft/esd:            0.00
 FE11     moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  ( 12) Values  : 0.540  0.333330  0.666670  0.214357    0.378
            Sigmas  :                             0.000048    0.005
            Shft/esd:                                0.00    -0.01

 FE+3  ( 12) Moments :           2.672     0.000     0.000    2.672   90.000    0.000
            Sigmas  :           0.042                        0.042    0.000    0.000
            Shft/esd:            0.00
 FE12     moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 2 :      0.01
 Calculated unit cell formula weight:   335.082, density:  1.694gm/cm**3

 Histogram scale factors:

 Histogram:    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 Scale    :    8.76047        8.76324        10.0664        0.00000        0.00000
 Sigmas   :   0.195805E-01   0.133022E-01   0.343969E-01    0.00000        0.00000
 Shift/esd:       0.03           0.05           0.01           0.00           0.00
 Histogram scale factor sum(shift/error)**2 :      0.00

 Lattice parameters for powder data:
 Phase  1
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202475  5.202475 14.014489    90.000    90.000   120.000     328.494
 Sigmas   :  0.000004  0.000004  0.000104     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Phase  2
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202432  5.202446 14.014500    90.000    90.000   119.999     328.494
 Sigmas   :  0.000007  0.000007  0.000104     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Recprocal metric tensor sum(shift/error)**2 :      0.00
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 Diffractometer coefficients for powder data:
 Histogram :    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 C/L1/R/2Th:    4569.20        6162.13        2139.59        0.00000        0.00000
 Sigmas    :   0.354173E-01    0.00000       0.493395E-01    0.00000        0.00000
 Shift/esd :      -0.01           0.00          -0.01           0.00           0.00
```

```
 Dif A/Pola:  -0.970497       -2.51000        1.29873        0.00000        0.00000
 Sigmas    :   0.222284E-01    0.00000       0.224534E-01    0.00000        0.00000
 Shift/esd :      -0.01           0.00          -0.01           0.00           0.00
 Zero      :    1.90000        3.85000        9.03000        0.00000        0.00000
 Sigmas    :    0.00000        0.00000        0.00000        0.00000        0.00000
 Shift/esd :      -0.01           0.00          -0.01           0.00           0.00
 Dif. Cons. Sum(shift/error)**2 :      0.00

 Profile coefficients for histogram no.  1 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.470E+01  2.080E+00  0.000E+00  3.129E+00  0.000E+00
0.000E+00
 Sigmas   :                                              4.847E-01                        7.620E-02
 Shift/esd:                                                 -0.01                             0.01
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.394E+01 -1.859E+00  0.000E+00  1.876E-02  1.628E+00
0.000E+00
 Sigmas   :                                              3.832E-01                        4.968E-02
 Shift/esd:                                                 -0.01                             0.02
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.318E-01
 Shift/esd:                                                  0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
1SFO                                                    GENLES   Version MacOSX Jun 14 18:25:47 2011
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 Profile coefficients for histogram no.  1 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.470E+01  2.080E+00  0.000E+00  3.129E+00  0.000E+00
0.000E+00
 Sigmas   :                                              4.847E-01                        7.620E-02
 Shift/esd:                                                 -0.01                             0.01
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
```

```
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.394E+01 -1.859E+00  0.000E+00  1.876E-02  1.628E+00
0.000E+00
 Sigmas   :                                              3.832E-01                        4.968E-02
 Shift/esd:                                                 -0.01                             0.02
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.318E-01
 Shift/esd:                                                  0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
 Profile coef. sum(shift/error)**2 :      0.00

 Background coefficients for histogram no.  1:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   3.310255E-01  -1.649298E-02   5.384265E-02  -1.737273E-02  -8.909297E-03  -3.880237E-02
 Sigmas   :   6.026207E-04   8.384967E-04   1.042680E-03   8.941597E-04   8.444989E-04   8.442348E-04
 Shift/esd:           0.01          -0.01           0.00          -0.01           0.00           0.00
 Param.   :           7             8             9
 Coeff.   :  -1.790377E-02  -1.493028E-02  -6.961925E-03
 Sigmas   :   8.422531E-04   8.461392E-04   8.279817E-04
 Shift/esd:           0.00           0.00          -0.01
1SFO                                                          GENLES   Version MacOSX Jun 14 18:25:47 2011
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 Background coefficients for histogram no.  2:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   2.739778E-01  -9.744284E-02   9.679380E-03  -1.750145E-02   1.120639E-02  -8.097776E-03
 Sigmas   :   3.743004E-04   4.858064E-04   6.158398E-04   5.772812E-04   5.432080E-04   5.315231E-04
 Shift/esd:           0.02          -0.02           0.01           0.00           0.00           0.00
 Param.   :           7             8             9            10            11            12
 Coeff.   :   3.169314E-04  -1.456465E-02  -6.478267E-03   2.394573E-03   3.947360E-03  -1.672721E-02
 Sigmas   :   5.307352E-04   5.276783E-04   5.248328E-04   5.165406E-04   5.124590E-04   5.124880E-04
 Shift/esd:           0.01           0.00           0.00          -0.01          -0.01           0.00
 Background coef. sum(shift/error)**2 :      0.00

 CPU times for matrix build     1.51 sec; matrix inversion     0.01 sec
 Final variable sum((shift/esd)**2) for cycle1156:       0.01 Time:    1.52 sec

 Convergence was achieved

-----------------------------------------------
     Archiving SAFE_NEUTRON_FINAL_STEPHANSS.EXP as SAFE_NEUTRON_FINAL_STEPHANSS.003
-----------------------------------------------
```

```
                  |----------------------------------------|
                  |     Program PUBTABLES Version MacOSX   |
                  |  Generate crystal structure data tables |
                  | Distributed on Wed Apr 21 18:37:08 2010 |
                  |----------------------------------------|

        |-------------------------------------------------------------|
        |            Allen C. Larson and Robert B. Von Dreele         |
        |      Manuel Lujan, Jr. Neutron Scattering Center, MS-H805    |
        |      Los Alamos National Laboratory, Los Alamos, NM  87545   |
        |                                                             |
        | Copyright, 2000, The Regents of the University of California. |
        |-------------------------------------------------------------|

 The last history record is :
     HSTRY 86 EXPGUI 1113 1033 (1 changes) -- 06/14/2011 18:26:17

-----------------------------------------------
     Archiving SAFE_NEUTRON_FINAL_STEPHANSS.EXP as SAFE_NEUTRON_FINAL_STEPHANSS.004
-----------------------------------------------


-----------------------------------------------
     Archiving SAFE_NEUTRON_FINAL_STEPHANSS.EXP as SAFE_NEUTRON_FINAL_STEPHANSS.005
-----------------------------------------------
```



```
           |-----------------------------------------------------|
           |              Program POWPREF Version Win32          |
           | Prepares powder histograms for least-squares refinement |
           |         Distributed on Wed Jun 01 16:54:26 2011     |
           |-----------------------------------------------------|

        |-------------------------------------------------------------|
        |            Allen C. Larson and Robert B. Von Dreele         |
        |      Manuel Lujan, Jr. Neutron Scattering Center, MS-H805    |
        |      Los Alamos National Laboratory, Los Alamos, NM  87545   |
        |                                                             |
        | Copyright, 2000, The Regents of the University of California. |
        |-------------------------------------------------------------|

 The last history record is :
     HSTRY 88 EXPGUI 1113 1033 (1 changes) -- 06/24/11 14:07:17
 Data for bank  1 read from file e56881.gsa
 The powder pattern has  4524 channels with   1 bins per channel
 Histogram weight factors are    1.00000        0.00000
 No fixed background points for this powder pattern
 The  2 excluded regions are (in msec):
 Exclude    from:       to:     from:       to:     from:       to:     from:       to:
           0.0000    2.0000   20.0000 1000.0000
 Incident spectrum type  0 can be used in the region    1.000 msec to   20.000 msec
 The minimum possible weighted residual for this histogram is   0.0689
 Histogram no.  1 on file SAFE_NEUTRON_FINAL_STEPHANSS.P01
 updated with new excluded regions, background and incident spectrum data.
 CPU time =   0.00 to update histogram
 Lattice parameters for phase 1 are:
  a,b,c  =  5.202475  5.202475 14.014489  angles =    90.000    90.000   120.000
  volume =     328.494
 Lattice parameters for phase 2 are:
  a,b,c  =  5.202432  5.202446 14.014500  angles =    90.000    90.000   119.999
  volume =     328.494
 Profile function  3 for phase no. 1 has the coefficients p1-p21:
    0.289766E+00   0.528838E-01   0.746764E-02   0.000000E+00
    0.247043E+02   0.208014E+01   0.000000E+00   0.312877E+01
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
```

```
   0.000000E+00
cutoff on the wings at 0.001 of maximum

Profile function  3 for phase no. 2 has the coefficients p1-p21:
   0.289766E+00   0.528838E-01   0.746764E-02   0.000000E+00
   0.247043E+02   0.208014E+01   0.000000E+00   0.312877E+01
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00

   0.000000E+00
cutoff on the wings at 0.001 of maximum

Minimum d-spacing used to generate reflections   0.4215 for phase 1
Minimum d-spacing used to generate reflections   0.4215 for phase 2
Minimum d-spacing used to generate reflections   0.9629 for phase 1
Minimum d-spacing used to generate reflections   0.9629 for phase 2
Minimum d-spacing for matching reflections   0.4370
Estimated number of reflections to be generated is  1760
Minimum d-spacing for magnetic reflections   1.0000
Est. number of magnetic reflections to be generated is   914
Number of reflections generated for phase 1 is   514
Number of reflections generated for phase 2 is   794
Total number of reflections generated for all phases is  1308
CPU time =   0.00 sec. to generate reflections.
CPU time =   0.20 sec. to locate reflection limits.
CPU time =   0.00 sec. to match reflection ranges to powder pattern
The maximum number of reflections contributing to any profile point is  204
CPU time =   0.00 sec. to update file
Data for bank  2 read from file c56881.gsa
The powder pattern has  3756 channels with   1 bins per channel
Histogram weight factors are    1.00000        0.00000
No fixed background points for this powder pattern
The  2 excluded regions are (in msec):
Exclude    from:       to:     from:       to:     from:       to:     from:       to:
          0.0000    2.9980   20.0000 1000.0000
Incident spectrum type  0 can be used in the region    1.000 msec to   20.000 msec
The number of zero intensities found in this histogram is    2
The minimum possible weighted residual for this histogram is   0.0391
Histogram no.  2 on file SAFE_NEUTRON_FINAL_STEPHANSS.P02
updated with new excluded regions, background and incident spectrum data.
CPU time =   0.00 to update histogram
Profile function  3 for phase no. 1 has the coefficients p1-p21:
   0.410819E+01   0.678940E-01   0.285702E-02   0.354299E+01
   0.439370E+02  -0.185852E+01   0.000000E+00   0.187598E-01
   0.162805E+01   0.000000E+00   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00

   0.000000E+00
cutoff on the wings at 0.001 of maximum

Profile function  3 for phase no. 2 has the coefficients p1-p21:
   0.410819E+01   0.678940E-01   0.285702E-02   0.354299E+01
   0.439370E+02  -0.185852E+01   0.000000E+00   0.187598E-01
   0.162805E+01   0.000000E+00   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
   0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00

   0.000000E+00
cutoff on the wings at 0.001 of maximum

Minimum d-spacing used to generate reflections   0.4738 for phase 1
Minimum d-spacing used to generate reflections   0.4738 for phase 2
Minimum d-spacing used to generate reflections   0.9765 for phase 1
Minimum d-spacing used to generate reflections   0.9765 for phase 2
Minimum d-spacing for matching reflections   0.4858
Estimated number of reflections to be generated is  1515
Minimum d-spacing for magnetic reflections   1.0000
Est. number of magnetic reflections to be generated is   878
Number of reflections generated for phase 1 is   359
Number of reflections generated for phase 2 is   734
Total number of reflections generated for all phases is  1093
CPU time =   0.02 sec. to generate reflections.
CPU time =   0.13 sec. to locate reflection limits.
CPU time =   0.02 sec. to match reflection ranges to powder pattern
```

```
 The maximum number of reflections contributing to any profile point is  106
 CPU time =   0.00 sec. to update file
 Data for bank  3 read from file a56881.gsa
 The powder pattern has  4821 channels with   1 bins per channel
 Histogram weight factors are    1.00000        0.00000
 No fixed background points for this powder pattern
 The  2 excluded regions are (in msec):
 Exclude    from:       to:     from:       to:     from:       to:     from:       to:
          0.0000    1.5520   20.0000 1000.0000
 Incident spectrum type  0 can be used in the region    0.500 msec to   20.000 msec
 The number of zero intensities found in this histogram is   13
 The minimum possible weighted residual for this histogram is   0.1351
 Histogram no.  3 on file SAFE_NEUTRON_FINAL_STEPHANSS.P03
 updated with new excluded regions, background and incident spectrum data.
 CPU time =   0.00 to update histogram
 Profile function  3 for phase no. 1 has the coefficients p1-p21:
    0.100000E+01   0.527857E-01   0.202603E+00   0.219247E+02
    0.786492E+02   0.128369E+01   0.000000E+00   0.000000E+00
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00

    0.000000E+00
 cutoff on the wings at 0.001 of maximum

 Profile function  3 for phase no. 2 has the coefficients p1-p21:
    0.100000E+01   0.527857E-01   0.202603E+00   0.219247E+02
    0.786492E+02   0.128369E+01   0.000000E+00   0.000000E+00
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00
    0.000000E+00   0.000000E+00   0.000000E+00   0.000000E+00

    0.000000E+00
 cutoff on the wings at 0.001 of maximum

 Minimum d-spacing used to generate reflections   0.7029 for phase 1
 Minimum d-spacing used to generate reflections   0.7029 for phase 2
 Minimum d-spacing used to generate reflections   0.9742 for phase 1
 Minimum d-spacing used to generate reflections   0.9742 for phase 2
 Minimum d-spacing for matching reflections   0.7206
 Estimated number of reflections to be generated is  1169
 Minimum d-spacing for magnetic reflections   1.0000
 Est. number of magnetic reflections to be generated is   884
 Number of reflections generated for phase 1 is   112
 Number of reflections generated for phase 2 is   746
 Total number of reflections generated for all phases is   858
 CPU time =   0.02 sec. to generate reflections.
 CPU time =   0.09 sec. to locate reflection limits.
 CPU time =   0.00 sec. to match reflection ranges to powder pattern
 The maximum number of reflections contributing to any profile point is  128
 CPU time =   0.00 sec. to update file
1SFO                                                                    Version        Jun 24 14:07:24 2011
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             |-----------------------------------------------------|
             |            Program GENLES Version Win32             |
             |    General crystal structure refinement program     |
             | Magnetic structure refinement added by M. Yethiraj  |
             |   Revised and corrected by Larson and Von Dreele    |
             |      Distributed on Wed Jun 01 16:54:23 2011        |
             |-----------------------------------------------------|

        |-------------------------------------------------------------|
        |            Allen C. Larson and Robert B. Von Dreele         |
        |      Manuel Lujan, Jr. Neutron Scattering Center, MS-H805   |
        |      Los Alamos National Laboratory, Los Alamos, NM  87545  |
        |                                                             |
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        |-------------------------------------------------------------|

 The experiment file is: SAFE_NEUTRON_FINAL_STEPHANSS.EXP
 The last history record is :
     HSTRY 89 POWPREF Win32  Jun 24 14:07:18 2011
 Maximum number of cycles is   99
 Marquardt factor for matrix inversion =  1.00
```

```
 I/SigI cut-off is  1.00
 Structure factors will be extracted from histogram  1
 using extraction method codes     0    0    0    0    0    0    0    0    0
 Structure factors will be extracted from histogram  2
 using extraction method codes     0    0    0    0    0    0    0    0    0
 Structure factors will be extracted from histogram  3
 using extraction method codes     0    0    0    0    0    0    0    0    0

 The atomic and magnetic scattering factors for  3 types of atoms are:
 Atom type   b-len     a(1)      b(1)      a(2)      b(2)      a(3)      b(3)      a(4)      b(4)      c
g
 SC+3        1.229   13.4008    0.2985    8.0273    7.9629    1.6594   -0.2860    1.5794   16.0662   -6.6667
 <j0> Mag. ff   :     0.5048   31.4040    0.5186   10.9900   -0.0241    1.1830    0.0000    0.0000    0.0000
 <j2> Mag. ff   :     4.3683   28.6540    3.7231   10.8230    0.6074    3.6680    0.0000    0.0000    0.0014
2.000
 FE+3        0.945   11.1764    4.6147    7.3863    0.3005    3.3948   11.6729    0.0724   38.5566    0.9707
 <j0> Mag. ff   :     0.3972   13.2440    0.6295    4.9030   -0.0314    0.3500    0.0000    0.0000    0.0044
 <j2> Mag. ff   :     1.3602   11.9980    1.5188    5.0030    0.4705    1.9910    0.0000    0.0000    0.0038
2.000
 O           0.580    3.0485   13.2771    2.2868    5.7011    1.5463    0.3239    0.8670   32.9089    0.2508
 Atom type      CrKa     FeKa     CuKa     MoKa     AgKa     TiKa     CoKa     TaKa      WKa      AuKa
 SC+3     f'   -0.694   -0.012    0.312    0.252    0.183   -5.426    0.147    0.016    0.013    0.002
          f"    2.965    2.256    1.533    0.372    0.235    4.002    1.977    0.034    0.032    0.023
 FE+3     f'   -1.294   -2.055   -1.134    0.346    0.289   -0.890   -3.331    0.044    0.039    0.017
          f"    0.762    0.565    3.197    0.844    0.545    1.052    0.490    0.084    0.079    0.058
 O        f'    0.093    0.072    0.049    0.011    0.006    0.121    0.063   -0.002   -0.003   -0.003
          f"    0.073    0.052    0.032    0.006    0.004    0.106    0.044    0.000    0.000    0.000
1SFO                                                              GENLES   Version Win32  Jun 24 14:07:24 2011
Page   2


 Space group  R 3 c
 The lattice is acentric  R-centered trigonal      Laue symmetry 3barm1
  Multiplicity of a general site is  18
  The location of the origin is arbitrary in z

 The equivalent positions are:

 ( 1)     X      Y      Z  ( 2)    -Y     X-Y     Z  ( 3)    Y-X    -X      Z
 ( 4)    Y-X     Y  1/2+Z  ( 5)    -Y     -X  1/2+Z  ( 6)     X     X-Y 1/2+Z


 The atom positions read in are: (all variable numbers (pn) are in hexadecimal)

 Type seq. At. name  mult   symm  frac   pn    X    pn    Y    pn    Z    pn  u11 pn  u22 pn  u33 pn  u12 pn  u13
pn  u23 pn
 SC+3    1 Sc1         6    3    0.4600   0 0.0000   0 0.0000   0 0.0477   1 0.4   2
 FE+3    2 Fe1         6    3    0.4600   0 0.0000   0 0.0000   0 0.2579   0 0.5   3
 O       3 O1         18    1    1.0000   0 0.3424   4-0.0260   5 0.8176   6 0.5   7
 FE+3    4 Fe2         6    3    0.5400   0 0.0000   0 0.0000   0 0.0477   8 0.4   9
 SC+3    5 Sc2         6    3    0.5400   0 0.0000   0 0.0000   0 0.2579   0 0.5   A

 Space group  P 1
 The lattice is acentric   primitive triclinic     Laue symmetry 1bar
  Multiplicity of a general site is   1
  The location of the origin is arbitrary in xyz

 The equivalent positions are:

 ( 1)     X      Y      Z

 Parameters to be held - 2  1MY   2  1MZ   2  2MY   2  2MZ   2  3MY   2  3MZ   2  4MY   2  4MZ
 Parameters to be held - 2  5MY   2  6MZ   2  7MZ   2  5MZ   2  6MY   2  7MY   2  8MY   2  8MZ
 Parameters to be held - 2  9MY   2  9MZ   2 10MY   2 10MZ   2 11MY   2 11MZ   2 12MZ   2 12MY
 Parameters to be held - 2  7X    2  7Y    2  8X    2  8Y    2  9X    2  9Y    2 10X    2 10Y
 Parameters to be held - 2 11X    2 11Y    2 12X    2 12Y

 All of the following data refer to the current space group symbol
 No antisymmetry operations are allowed

 The atom positions read in are: (all variable numbers (pn) are in hexadecimal)

 Type seq. At. name  mult   symm  frac   pn    X    pn    Y    pn    Z    pn  u11 pn  u22 pn  u33 pn  u12 pn  u13
pn  u23 pn
                                          Mx    pn   My    pn   Mz    pn
 FE+3    1 FE1         1    1    0.4600   0 0.0000   0 0.0000   0 0.2579   0 0.5   B
```

```
                                          2.672  C   0.000  0   0.000  0
 FE+3    2 FE2         1    1    0.4600   0 0.6667   0 0.3333   0 0.5912   0 0.5   D
                                          2.672  E   0.000  0   0.000  0
 FE+3    3 FE3         1    1    0.4600   0 0.3333   0 0.6667   0 0.9246   0 0.5   F
                                          2.672 10   0.000  0   0.000  0
 FE+3    4 FE4         1    1    0.4600   0 0.0000   0 0.0000   0 0.7579   0 0.5  11
                                         -2.672 12   0.000  0   0.000  0
 FE+3    5 FE5         1    1    0.4600   0 0.6667   0 0.3333   0 0.0912   0 0.5  13
                                         -2.672 14   0.000  0   0.000  0
 FE+3    6 FE6         1    1    0.4600   0 0.3333   0 0.6667   0 0.4246   0 0.5  15
                                         -2.672 16   0.000  0   0.000  0
 FE+3    7 FE7         1    1    0.5400   0 0.0000   0 0.0000   0 0.0477  17 0.4  18
                                         -2.672 19   0.000  0   0.000  0
 FE+3    8 FE8         1    1    0.5400   0 0.6667   0 0.3333   0 0.3810  1A 0.4  1B
                                         -2.672 1C   0.000  0   0.000  0
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 The atom positions read in are: (all variable numbers (pn) are in hexadecimal)

 Type seq. At. name  mult   symm  frac   pn    X    pn    Y    pn    Z    pn  u11 pn  u22 pn  u33 pn  u12 pn  u13
pn  u23 pn
                                          Mx    pn   My    pn   Mz    pn
 FE+3    9 FE9         1    1    0.5400   0 0.3333   0 0.6667   0 0.7144  1D 0.4  1E
                                         -2.672 1F   0.000  0   0.000  0
 FE+3   10 FE10        1    1    0.5400   0 0.0000   0 0.0000   0 0.5477  20 0.4  21
                                          2.672 22   0.000  0   0.000  0
 FE+3   11 FE11        1    1    0.5400   0 0.6667   0 0.3333   0 0.8810  23 0.4  24
                                          2.672 25   0.000  0   0.000  0
 FE+3   12 FE12        1    1    0.5400   0 0.3333   0 0.6667   0 0.2144  26 0.4  27
                                          2.672 28   0.000  0   0.000  0
  Constraints read are LNCN   1 1  1Z     1.0000 1  4Z     1.0000 2  7Z     1.0000 2  8Z     1.0000
                       LNCN   1 2  9Z     1.0000 2 10Z     1.0000 2 11Z     1.0000 2 12Z     1.0000
                       LNCN   2 1  1FRAC -1.0000 1  2FRAC -1.0000 1  4FRAC  1.0000 1  5FRAC  1.0000
 Parameter missing - 1  1FRAC
 Parameter missing - 1  2FRAC
 Parameter missing - 1  4FRAC
 Parameter missing - 1  5FRAC
                       LNCN   2 2  1FRAC -1.0000 2  2FRAC -1.0000 2  3FRAC -1.0000 2  4FRAC -1.0000
 Parameter missing - 2  1FRAC
 Parameter missing - 2  2FRAC
 Parameter missing - 2  3FRAC
 Parameter missing - 2  4FRAC
                       LNCN   2 2  5FRAC -1.0000 2  6FRAC -1.0000 2  7FRAC  1.0000 2  8FRAC  1.0000
 Parameter missing - 2  5FRAC
 Parameter missing - 2  6FRAC
 Parameter missing - 2  7FRAC
 Parameter missing - 2  8FRAC
                       LNCN   2 2  9FRAC  1.0000 2 10FRAC  1.0000 2 11FRAC  1.0000 2 12FRAC  1.0000
 Parameter missing - 2  9FRAC
 Parameter missing - 2 10FRAC
 Parameter missing - 2 11FRAC
 Parameter missing - 2 12FRAC
                       LNCN   3 1  2Z     1.0000 1  5Z     1.0000 2  1Z     1.0000 2  2Z     1.0000
 Parameter missing - 1  2Z
 Parameter missing - 1  5Z
 Parameter missing - 2  1Z
 Parameter missing - 2  2Z
                       LNCN   3 2  3Z     1.0000 2  4Z     1.0000 2  5Z     1.0000 2  6Z     1.0000
 Parameter missing - 2  3Z
 Parameter missing - 2  4Z
 Parameter missing - 2  5Z
 Parameter missing - 2  6Z
                       LNCN   4 1  1UISO  1.0000 1  4UISO  1.0000 2  7UISO  1.0000 2  8UISO  1.0000
                       LNCN   4 2  9UISO  1.0000 2 10UISO  1.0000 2 11UISO  1.0000 2 12UISO  1.0000
                       LNCN   5 2  1MX    1.0000 2  2MX    1.0000 2  3MX    1.0000 2 10MX    1.0000
                       LNCN   5 2 11MX    1.0000 2 12MX    1.0000 2  4MX   -1.0000 2  5MX   -1.0000
                       LNCN   5 2  6MX   -1.0000 2  7MX   -1.0000 2  8MX   -1.0000 2  9MX   -1.0000
                       LNCN   6 1  2UISO  1.0000 1  5UISO  1.0000 2  1UISO  1.0000 2  2UISO  1.0000
                       LNCN   6 2  3UISO  1.0000 2  4UISO  1.0000 2  5UISO  1.0000 2  6UISO  1.0000
 Constraint no.  1 for type RMTN:   1    RM33     1.0000 2    RM33     1.0000
 Constraint no.  2 for type RMTN:   1    RM11     1.0000 2    RM11     1.0000 2    RM22     1.0000
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```

```
 Lattice parameters for phase 1 are:
     a          b          c          alpha      beta     gamma
    5.202475   5.202475  14.014489   90.0000   90.0000  120.0000
 These cell parameters will be refined
 Reciprocal metric tensor elements:          damp= 0
 Element :          g11   pn          g22   pn          g33   pn        2*g12   pn        2*g13   pn        2*g23
pn
 Value   :   4.92628E-02  29   4.92628E-02  2A   5.09150E-03  2B   4.92628E-02  2C  -6.67561E-10   0
-6.67561E-10   0
 Constr. :          1.000  2          1.000  2          1.000  2          1.000  2          0.000  0
0.000  0

 Lattice parameters for phase 2 are:
     a          b          c          alpha      beta     gamma
    5.202432   5.202446  14.014500   90.0000   90.0000  119.9987
 These cell parameters will be refined
 Reciprocal metric tensor elements:          damp= 0
 Element :          g11   pn          g22   pn          g33   pn        2*g12   pn        2*g13   pn        2*g23
pn
 Value   :   4.92623E-02  2D   4.92620E-02  2E   5.09149E-03  2F   4.92602E-02   0  -6.67539E-10   0
-6.67538E-10   0
 Constr. :          1.000  2          1.000  2          1.000  2          1.000  0          1.000  0
1.000  0

 Phase/element fractions for phase no.  1

 Hist Elm:    PNT   1 1   nc    PNT   2 1   nc    PNT   3 1   nc    PNT*  4 1   nc    PXC*  5 1   nc
 Fraction:    1.0000       0    1.0000       0    1.0000       0   not present       not present
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0

 Phase/element fractions for phase no.  2

 Hist Elm:    PNT   1 1   nc    PNT   2 1   nc    PNT   3 1   nc    PNT*  4 1   nc    PXC*  5 1   nc
 Fraction:    1.0000       0    1.0000       0    1.0000       0   not present       not present
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0

 Histogram scale factors:

 Hist/Typ:    1  PNT      pn    2  PNT      pn    3  PNT      pn    4  PNT*     pn    5  PXC*     pn
 Scale   :    8.7605      30    8.7632      31    10.066      32    0.0000       0    0.0000       0
 Dmp/Cnst:    0     1.000  3    0     1.000  4    0     1.000  5    0     0.000  0    0     0.000  0

 Absorption coefficients for powder data:

 Hist/Typ:    1  PNT    0 pn    2  PNT    0 pn    3  PNT    0 pn    4  PNT*   0 pn    5  PXC*   0 pn
 Absc 1. :   0.21758E-01   0   0.21758E-01   0   0.21758E-01   0    0.0000       0    0.0000       0
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0
 Absc 2. :    0.0000       0    0.0000       0    0.0000       0    0.0000       0    0.0000       0
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0
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 Diffractometer constants for powder data:
 No. Type    Dif C   pn    Dif A   pn     Zero   pn Cnstr  cn Damp
  1  PNT    4569.20  33     -0.97  35     1.900   0 0.000   0    0
 No. Type    Dif C   pn    Dif A   pn     Zero   pn Cnstr  cn Damp
  2  PNT    6162.13   0     -2.51   0     3.850   0 0.000   0    0
 No. Type    Dif C   pn    Dif A   pn     Zero   pn Cnstr  cn Damp
  3  PNT    2139.59  34      1.30  36     9.030   0 0.000   0    0

 Extinction coefficients for phase no.  1:

 Hist/Typ:    1  PNT      pn    2  PNT      pn    3  PNT      pn    4  PNT*     pn    5  PXC*     pn
 Extinct.:    0.0000       0    0.0000       0    0.0000       0    0.0000       0    0.0000       0
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0

 Extinction coefficients for phase no.  2:

 Hist/Typ:    1  PNT      pn    2  PNT      pn    3  PNT      pn    4  PNT*     pn    5  PXC*     pn
 Extinct.:    0.0000       0    0.0000       0    0.0000       0    0.0000       0   not present
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0

 Radiation damage coefficients for phase no.  1:
```

```
 Hist/Typ:    1  PNT      pn    2  PNT      pn    3  PNT      pn    4  PNT*     pn    5  PXC*     pn
 Rad.dam.:    0.0000       0    0.0000       0    0.0000       0    0.0000       0    0.0000       0
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0

 Radiation damage coefficients for phase no.  2:

 Hist/Typ:    1  PNT      pn    2  PNT      pn    3  PNT      pn    4  PNT*     pn    5  PXC*     pn
 Rad.dam.:    0.0000       0    0.0000       0    0.0000       0    0.0000       0   not present
 Dmp/Cnst:    0     0.000  0    0     0.000  0    0     0.000  0    0     0.000  0

 Preferred orientation coeffs. for phase no.  1 histogram no.  1:
 Axis    :        1       pn
 Dir./typ:    0.0 0.0 1.0  0
 PO ratio:        1.0000   0
 Dmp/Cnst:    0     0.000  0
 PO frac.:        1.0000   0
 Dmp/Cnst:    0     0.000  0
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 Preferred orientation coeffs. for phase no.  1 histogram no.  2:
 Axis    :        1       pn
 Dir./typ:    0.0 0.0 1.0  0
 PO ratio:        1.0000   0
 Dmp/Cnst:    0     0.000  0
 PO frac.:        1.0000   0
 Dmp/Cnst:    0     0.000  0

 Preferred orientation coeffs. for phase no.  1 histogram no.  3:
 Axis    :        1       pn
 Dir./typ:    0.0 0.0 1.0  0
 PO ratio:        1.0000   0
 Dmp/Cnst:    0     0.000  0
 PO frac.:        1.0000   0
 Dmp/Cnst:    0     0.000  0

 Preferred orientation coeffs. for phase no.  2 histogram no.  1:
 Axis    :        1       pn
 Dir./typ:    0.0 0.0 1.0  0
 PO ratio:        1.0000   0
 Dmp/Cnst:    0     0.000  0
 PO frac.:        1.0000   0
 Dmp/Cnst:    0     0.000  0

 Preferred orientation coeffs. for phase no.  2 histogram no.  2:
 Axis    :        1       pn
 Dir./typ:    0.0 0.0 1.0  0
 PO ratio:        1.0000   0
 Dmp/Cnst:    0     0.000  0
 PO frac.:        1.0000   0
 Dmp/Cnst:    0     0.000  0

 Preferred orientation coeffs. for phase no.  2 histogram no.  3:
 Axis    :        1       pn
 Dir./typ:    0.0 0.0 1.0  0
 PO ratio:        1.0000   0
 Dmp/Cnst:    0     0.000  0
 PO frac.:        1.0000   0
 Dmp/Cnst:    0     0.000  0


 Constraint no.  1 for type PF 5:   ALL,1         1.000
 Constraint no.  2 for type PF 5:   ALL,2         1.000
 Constraint no.  3 for type PF 5:   ALL,3         1.000

 Constraint no.  1 for type PF 8:   ALL,1         1.000
 Constraint no.  2 for type PF 8:   ALL,2         1.000
 Constraint no.  3 for type PF 8:   ALL,3         1.000
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 Profile coeff. for function type  3, phase no.  1 and histogram no.  1; aniso. axis   0.   0.   1.; damp= 0:
 Coeff.  :     alp    pn     be-0   pn     be-1   pn     sg-0   pn     sg-1   pn     sg-2   pn     ga-0   pn
ga-1   pn
```

```
 Value   : 2.898E-01   0 5.288E-02   0 7.468E-03   0 0.000E+00   0 2.470E+01  37 2.080E+00   0 0.000E+00   0
3.129E+00  3D
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      1.000 10      0.000  0      0.000  0
1.000 13
 Coeff.  :     ga-2   pn     gsf    pn     g1ec   pn     g2ec   pn     rstr   pn     rsta   pn     rsca   pn
L11    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
0.000  0
 Coeff.  :     L22    pn     L33    pn     L12    pn     L13    pn     L23    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0

 Profile coeff. for function type  3, phase no.  1 and histogram no.  2; aniso. axis   0.   0.   1.; damp= 0:
 Coeff.  :     alp    pn     be-0   pn     be-1   pn     sg-0   pn     sg-1   pn     sg-2   pn     ga-0   pn
ga-1   pn
 Value   : 4.108E+00   0 6.789E-02   0 2.857E-03   0 3.543E+00   0 4.394E+01  38-1.859E+00   0 0.000E+00   0
1.876E-02  3E
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      1.000 11      0.000  0      0.000  0
1.000 14
 Coeff.  :     ga-2   pn     gsf    pn     g1ec   pn     g2ec   pn     rstr   pn     rsta   pn     rsca   pn
L11    pn
 Value   : 1.628E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
0.000  0
 Coeff.  :     L22    pn     L33    pn     L12    pn     L13    pn     L23    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0

 Profile coeff. for function type  3, phase no.  1 and histogram no.  3; aniso. axis   0.   0.   1.; damp= 0:
 Coeff.  :     alp    pn     be-0   pn     be-1   pn     sg-0   pn     sg-1   pn     sg-2   pn     ga-0   pn
ga-1   pn
 Value   : 1.000E+00   0 5.279E-02   0 2.026E-01   0 2.192E+01   0 7.865E+01  39 1.284E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      1.000 12      0.000  0      0.000  0
0.000  0
 Coeff.  :     ga-2   pn     gsf    pn     g1ec   pn     g2ec   pn     rstr   pn     rsta   pn     rsca   pn
L11    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
0.000  0
 Coeff.  :     L22    pn     L33    pn     L12    pn     L13    pn     L23    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0

 Profile coeff. for function type  3, phase no.  2 and histogram no.  1; aniso. axis   0.   0.   1.; damp= 0:
 Coeff.  :     alp    pn     be-0   pn     be-1   pn     sg-0   pn     sg-1   pn     sg-2   pn     ga-0   pn
ga-1   pn
 Value   : 2.898E-01   0 5.288E-02   0 7.468E-03   0 0.000E+00   0 2.470E+01  3A 2.080E+00   0 0.000E+00   0
3.129E+00  3F
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      1.000 10      0.000  0      0.000  0
1.000 13
 Coeff.  :     ga-2   pn     gsf    pn     g1ec   pn     g2ec   pn     rstr   pn     rsta   pn     rsca   pn
L11    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
0.000  0
 Coeff.  :     L22    pn     L33    pn     L12    pn     L13    pn     L23    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0

 Profile coeff. for function type  3, phase no.  2 and histogram no.  2; aniso. axis   0.   0.   1.; damp= 0:
 Coeff.  :     alp    pn     be-0   pn     be-1   pn     sg-0   pn     sg-1   pn     sg-2   pn     ga-0   pn
ga-1   pn
 Value   : 4.108E+00   0 6.789E-02   0 2.857E-03   0 3.543E+00   0 4.394E+01  3B-1.859E+00   0 0.000E+00   0
1.876E-02  40
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      1.000 11      0.000  0      0.000  0
1.000 14
 Coeff.  :     ga-2   pn     gsf    pn     g1ec   pn     g2ec   pn     rstr   pn     rsta   pn     rsca   pn
L11    pn
 Value   : 1.628E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
0.000E+00   0
```

```
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
0.000  0
 Coeff.  :     L22    pn     L33    pn     L12    pn     L13    pn     L23    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
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 Profile coeff. for function type  3, phase no.  2 and histogram no.  3; aniso. axis   0.   0.   1.; damp= 0:
 Coeff.  :     alp    pn     be-0   pn     be-1   pn     sg-0   pn     sg-1   pn     sg-2   pn     ga-0   pn
ga-1   pn
 Value   : 1.000E+00   0 5.279E-02   0 2.026E-01   0 2.192E+01   0 7.865E+01  3C 1.284E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      1.000 12      0.000  0      0.000  0
0.000  0
 Coeff.  :     ga-2   pn     gsf    pn     g1ec   pn     g2ec   pn     rstr   pn     rsta   pn     rsca   pn
L11    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0
0.000  0
 Coeff.  :     L22    pn     L33    pn     L12    pn     L13    pn     L23    pn
 Value   : 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0 0.000E+00   0
 Constr. :      0.000  0      0.000  0      0.000  0      0.000  0      0.000  0

 Diffuse scattering coefficients for powder data:
 No diffuse scattering coefficients for histogram    1
 No diffuse scattering coefficients for histogram    2
 No diffuse scattering coefficients for histogram    3

 Background coefficients for powder data:
 Histogram no.:    1 Damping factor:    0 Use all points: Y
 Shifted Chebyshev function of first kind
 Param.  :          1   pn          2   pn          3   pn          4   pn          5   pn          6   pn
 Coeff.  : 0.33103E+00  41-0.16493E-01  43 0.53843E-01  45-0.17373E-01  47-0.89093E-02  49-0.38802E-01  4B
 Param.  :          7   pn          8   pn          9   pn
 Coeff.  :-0.17904E-01  4D-0.14930E-01  4F-0.69619E-02  51
 Histogram no.:    2 Damping factor:    0 Use all points: Y
 Shifted Chebyshev function of first kind
 Param.  :          1   pn          2   pn          3   pn          4   pn          5   pn          6   pn
 Coeff.  : 0.27398E+00  42-0.97443E-01  44 0.96794E-02  46-0.17501E-01  48 0.11206E-01  4A-0.80978E-02  4C
 Param.  :          7   pn          8   pn          9   pn         10   pn         11   pn         12   pn
 Coeff.  : 0.31693E-03  4E-0.14565E-01  50-0.64783E-02  52 0.23946E-02  53 0.39474E-02  54-0.16727E-01  55
 Histogram no.:    3 Damping factor:    0 Use all points: Y
 Shifted Chebyshev function of first kind
 Param.  :          1   pn          2   pn          3   pn          4   pn          5   pn          6   pn
 Coeff.  : 0.29912E+00   0-0.31899E-01   0-0.42900E-02   0-0.15951E-01   0 0.19462E-01   0-0.11893E-01   0
 Param.  :          7   pn          8   pn          9   pn         10   pn
 Coeff.  :-0.25533E-01   0 0.40060E-02   0 0.13208E-01   0-0.14414E-01   0

 The constraint matrix has     85 terms
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 Restraint data statistics:
 No restraints used

 Powder data statistics                Fitted         -Bknd          pFree                 Average
              Bank Ndata Sum(w*d**2)  wRp     Rp    wRp     Rp    wRp     Rp  Npfree  DWd  Integral
 Hstgm  1 PNT   1  4524  4595.3     0.0694 0.1158 3.0673 0.6237 0.0000 0.0000     0   0.658   0.982
 Hstgm  2 PNT   2  3753  4939.8     0.0449 0.0942 0.1097 0.1131 0.0000 0.0000     0   0.462   0.990
 Hstgm  3 PNT   3  4808  4302.6     0.1278 0.1742 3.2083 0.7146 0.0000 0.0000     0   0.733   0.997
 Powder totals    13085  13838.     0.0614 0.1235 1.9262 0.4499 0.0000 0.0000     0   0.611

 No serial correlation in fit at 90% confidence for 1.952 < DWd < 2.048
 Cycle1157 There were  13085 observations.
 Total before-cycle CHI**2 (offset/sig) = 1.3838E+04 ( 4.9265E+00)
 Reduced CHI**2 =  1.061     for   43 variables

 Reflection data statistics
 Histogram  1  Type PNT   Nobs = 1302 R(F**2) =  0.1131
 Histogram  2  Type PNT   Nobs = 1071 R(F**2) =  0.0970
 Histogram  3  Type PNT   Nobs =  857 R(F**2) =  0.0802
 After matrix normalization and Marquardt modification:
```

```
   1 Columns of the    43 Column matrix are 0.0
 Full matrix recip. condition value & -log10 =   0.2038E-03      3.69
        Variable NoVarabl was not refined

 The value of the determinant is  1.2658*10.0**(   -22)

 Atom parameters for phase no. 1
                    frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
 SC+3  (  1) Values  : 0.460  0.000000  0.000000  0.047674    0.347
             Sigmas  :                             0.000050    0.033
             Shft/esd:                               -0.25    -0.94
 Sc1      moved  0.00A     sum(shift/e.s.d)**2 :    0.95

 FE+3  (  2) Values  : 0.460  0.000000  0.000000  0.257903    0.548
             Sigmas  :                                       0.036
             Shft/esd:                                        1.05
 Fe1      moved  0.00A     sum(shift/e.s.d)**2 :    1.10

 O     (  3) Values  : 1.000  0.342321 -0.026074  0.817598    0.487
             Sigmas  :        0.000384  0.000225  0.000225    0.010
             Shft/esd:          -0.28     -0.25      0.10     0.51
 O1       moved  0.00A     sum(shift/e.s.d)**2 :    0.41

 FE+3  (  4) Values  : 0.540  0.000000  0.000000  0.047674    0.347
             Sigmas  :                             0.000050    0.033
             Shft/esd:                               -0.25    -0.94
 Fe2      moved  0.00A     sum(shift/e.s.d)**2 :    0.95

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 SC+3  (  5) Values  : 0.540  0.000000  0.000000  0.257903    0.548
             Sigmas  :                                       0.036
             Shft/esd:                                        1.05
 Sc2      moved  0.00A     sum(shift/e.s.d)**2 :    1.10

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 1 :      4.53
 Calculated unit cell formula weight:   892.800, density:  4.513gm/cm**3

 Atom parameters for phase no. 2
                    frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
                                 Mx        My        Mz     |Moment|   Theta    Psi
 FE+3  (  1) Values  : 0.460  0.000000  0.000000  0.257890    0.548
             Sigmas  :                                       0.036
             Shft/esd:                                        1.05

 FE+3  (  1) Moments :           2.669     0.000     0.000    2.669   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:           -0.05
 FE1      moved  0.00A     sum(shift/e.s.d)**2 :    1.11

 FE+3  (  2) Values  : 0.460  0.666670  0.333330  0.591220    0.548
             Sigmas  :                                       0.036
             Shft/esd:                                        1.05

 FE+3  (  2) Moments :           2.669     0.000     0.000    2.669   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:           -0.05
 FE2      moved  0.00A     sum(shift/e.s.d)**2 :    1.11

 FE+3  (  3) Values  : 0.460  0.333330  0.666670  0.924560    0.548
             Sigmas  :                                       0.036
             Shft/esd:                                        1.05

 FE+3  (  3) Moments :           2.669     0.000     0.000    2.669   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:           -0.05
 FE3      moved  0.00A     sum(shift/e.s.d)**2 :    1.11

 FE+3  (  4) Values  : 0.460  0.000000  0.000000  0.757890    0.548
             Sigmas  :                                       0.036
             Shft/esd:                                        1.05
```

```
 FE+3  (  4) Moments :          -2.669     0.000     0.000    2.669   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.05
 FE4       moved  0.00A     sum(shift/e.s.d)**2 :    1.11

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 FE+3  (  5) Values  : 0.460  0.666670  0.333330  0.091220    0.548
              Sigmas  :                                      0.036
              Shft/esd:                                       1.05

 FE+3  (  5) Moments :          -2.669     0.000     0.000    2.669   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.05
 FE5       moved  0.00A     sum(shift/e.s.d)**2 :    1.11

 FE+3  (  6) Values  : 0.460  0.333330  0.666670  0.424560    0.548
              Sigmas  :                                      0.036
              Shft/esd:                                       1.05

 FE+3  (  6) Moments :          -2.669     0.000     0.000    2.669   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.05
 FE6       moved  0.00A     sum(shift/e.s.d)**2 :    1.11

 FE+3  (  7) Values  : 0.540  0.000000  0.000000  0.047674    0.347
              Sigmas  :                              0.000050    0.033
              Shft/esd:                                 -0.25    -0.94

 FE+3  (  7) Moments :          -2.669     0.000     0.000    2.669   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.05
 FE7       moved  0.00A     sum(shift/e.s.d)**2 :    0.96

 FE+3  (  8) Values  : 0.540  0.666670  0.333330  0.381004    0.347
              Sigmas  :                              0.000050    0.033
              Shft/esd:                                 -0.25    -0.94

 FE+3  (  8) Moments :          -2.669     0.000     0.000    2.669   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.05
 FE8       moved  0.00A     sum(shift/e.s.d)**2 :    0.96

 FE+3  (  9) Values  : 0.540  0.333330  0.666670  0.714345    0.347
              Sigmas  :                              0.000050    0.033
              Shft/esd:                                 -0.25    -0.94

 FE+3  (  9) Moments :          -2.669     0.000     0.000    2.669   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.05
 FE9       moved  0.00A     sum(shift/e.s.d)**2 :    0.96

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 FE+3  ( 10) Values  : 0.540  0.000000  0.000000  0.547675    0.347
              Sigmas  :                              0.000050    0.033
              Shft/esd:                                 -0.25    -0.94

 FE+3  ( 10) Moments :           2.669     0.000     0.000    2.669   90.000    0.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:           -0.05
 FE10      moved  0.00A     sum(shift/e.s.d)**2 :    0.96

 FE+3  ( 11) Values  : 0.540  0.666670  0.333330  0.881005    0.347
              Sigmas  :                              0.000050    0.033
              Shft/esd:                                 -0.25    -0.94

 FE+3  ( 11) Moments :           2.669     0.000     0.000    2.669   90.000    0.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:           -0.05
 FE11      moved  0.00A     sum(shift/e.s.d)**2 :    0.96

 FE+3  ( 12) Values  : 0.540  0.333330  0.666670  0.214345    0.347
```

```
            Sigmas  :                            0.000050    0.033
            Shft/esd:                               -0.25    -0.94

 FE+3  ( 12) Moments :           2.669     0.000     0.000    2.669   90.000    0.000
            Sigmas  :           0.043                         0.043    0.000    0.000
            Shft/esd:           -0.05
 FE12     moved  0.00A     sum(shift/e.s.d)**2 :    0.96

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 2 :     12.37
 Calculated unit cell formula weight:   335.082, density:  1.694gm/cm**3

 Histogram scale factors:

 Histogram:    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 Scale    :    8.77364        8.78160        10.0729        0.00000        0.00000
 Sigmas   :   0.331102E-01   0.299171E-01   0.362231E-01    0.00000        0.00000
 Shift/esd:       0.40           0.62           0.19           0.00           0.00
 Histogram scale factor sum(shift/error)**2 :      0.57

 Lattice parameters for powder data:
 Phase  1
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202475  5.202475 14.014489    90.000    90.000   120.000     328.494
 Sigmas   :  0.000004  0.000004  0.000114     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Phase  2
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202432  5.202446 14.014500    90.000    90.000   119.999     328.494
 Sigmas   :  0.000007  0.000007  0.000114     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Recprocal metric tensor sum(shift/error)**2 :      0.00
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 Diffractometer coefficients for powder data:
 Histogram :    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 C/L1/R/2Th:    4569.20        6162.13        2139.59        0.00000        0.00000
 Sigmas    :   0.105500        0.00000       0.153601        0.00000        0.00000
 Shift/esd :      -0.03           0.00           0.02           0.00           0.00
 Dif A/Pola:  -0.970336       -2.51000        1.29519        0.00000        0.00000
 Sigmas    :   0.627906E-01    0.00000       0.698688E-01    0.00000        0.00000
 Shift/esd :      -0.03           0.00           0.02           0.00           0.00
 Zero      :    1.90000        3.85000        9.03000        0.00000        0.00000
 Sigmas    :    0.00000        0.00000        0.00000        0.00000        0.00000
 Shift/esd :      -0.03           0.00           0.02           0.00           0.00
 Dif. Cons. Sum(shift/error)**2 :      0.01

 Profile coefficients for histogram no.  1 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.459E+01  2.080E+00  0.000E+00  3.152E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.529E-01                        1.562E-01
 Shift/esd:                                                 -0.14                            0.15
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.378E+01 -1.859E+00  0.000E+00  4.640E-02  1.628E+00
0.000E+00
 Sigmas   :                                              7.595E-01                        1.184E-01
 Shift/esd:                                                 -0.21                            0.23
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
```

```
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                             8.472E-01
 Shift/esd:                                                  0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
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 Profile coefficients for histogram no.  1 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.459E+01  2.080E+00  0.000E+00  3.152E+00  0.000E+00
0.000E+00
 Sigmas   :                                             8.529E-01                        1.562E-01
 Shift/esd:                                                -0.14                             0.15
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.378E+01 -1.859E+00  0.000E+00  4.640E-02  1.628E+00
0.000E+00
 Sigmas   :                                             7.595E-01                        1.184E-01
 Shift/esd:                                                -0.21                             0.23
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                             8.472E-01
 Shift/esd:                                                  0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
```

```
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
 Profile coef. sum(shift/error)**2 :      0.17

 Background coefficients for histogram no.  1:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   3.303978E-01  -1.781840E-02   5.272586E-02  -1.853620E-02  -9.874714E-03  -3.959066E-02
 Sigmas   :   4.614085E-03   8.662024E-03   7.904008E-03   7.311982E-03   6.852584E-03   6.160843E-03
 Shift/esd:          -0.14          -0.15          -0.14          -0.16          -0.14          -0.13
 Param.   :           7             8             9
 Coeff.   :  -1.858330E-02  -1.533384E-02  -7.153702E-03
 Sigmas   :   5.221982E-03   3.640774E-03   1.897049E-03
 Shift/esd:          -0.13          -0.11          -0.10
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 Background coefficients for histogram no.  2:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   2.736499E-01  -9.806749E-02   9.463286E-03  -1.771650E-02   1.122380E-02  -8.165664E-03
 Sigmas   :   2.500222E-03   4.625665E-03   4.215699E-03   3.986135E-03   3.837732E-03   3.727080E-03
 Shift/esd:          -0.13          -0.14          -0.05          -0.05           0.00          -0.02
 Param.   :           7             8             9            10            11            12
 Coeff.   :   1.238967E-04  -1.504364E-02  -7.065465E-03   1.783769E-03   3.499292E-03  -1.700513E-02
 Sigmas   :   3.603243E-03   3.500275E-03   3.258536E-03   2.870727E-03   2.146273E-03   1.151718E-03
 Shift/esd:          -0.05          -0.14          -0.18          -0.21          -0.21          -0.24
 Background coef. sum(shift/error)**2 :      0.34

 CPU times for matrix build     1.55 sec; matrix inversion     0.00 sec
 Final variable sum((shift/esd)**2) for cycle1157:       3.60 Time:    1.55 sec
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 Restraint data statistics:
 No restraints used

 Powder data statistics                Fitted         -Bknd          pFree                  Average
              Bank Ndata Sum(w*d**2)  wRp     Rp    wRp     Rp    wRp     Rp  Npfree  DWd  Integral
 Hstgm  1 PNT   1  4524  4592.7     0.0694 0.1159 3.0071 0.6136 0.0000 0.0000     0   0.658   0.982
 Hstgm  2 PNT   2  3753  4940.6     0.0449 0.0945 0.1091 0.1136 0.0000 0.0000     0   0.462   0.990
 Hstgm  3 PNT   3  4808  4303.4     0.1278 0.1742 3.2083 0.7146 0.0000 0.0000     0   0.732   0.997
 Powder totals    13085  13837.     0.0614 0.1237 1.9001 0.4462 0.0000 0.0000     0   0.611

 No serial correlation in fit at 90% confidence for 1.952 < DWd < 2.048
 Cycle1158 There were  13085 observations.
 Total before-cycle CHI**2 (offset/sig) = 1.3837E+04 ( 4.9211E+00)
 Reduced CHI**2 =  1.061     for   43 variables

 Reflection data statistics
 Histogram  1  Type PNT   Nobs = 1302 R(F**2) =  0.1149
 Histogram  2  Type PNT   Nobs = 1071 R(F**2) =  0.0983
 Histogram  3  Type PNT   Nobs =  857 R(F**2) =  0.0804
 After matrix normalization and Marquardt modification:

    1 Columns of the    43 Column matrix are 0.0
 Full matrix recip. condition value & -log10 =   0.2033E-03      3.69
         Variable NoVarabl was not refined

 The value of the determinant is  1.3370*10.0**(   -22)

 Atom parameters for phase no. 1
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
 SC+3  (  1) Values  : 0.460  0.000000  0.000000  0.047682    0.370
             Sigmas  :                            0.000050    0.031
             Shft/esd:                               0.17     0.76
 Sc1      moved  0.00A     sum(shift/e.s.d)**2 :    0.61

 FE+3  (  2) Values  : 0.460  0.000000  0.000000  0.257903    0.521
             Sigmas  :                                       0.035
```

```
            Shft/esd:                                          -0.74
 Fe1      moved  0.00A     sum(shift/e.s.d)**2 :    0.55

 O     (  3) Values  : 1.000  0.342333 -0.026070  0.817557    0.485
            Sigmas  :        0.000390  0.000228  0.000227    0.010
            Shft/esd:           0.03      0.02     -0.18    -0.12
 O1       moved  0.00A     sum(shift/e.s.d)**2 :    0.05

 FE+3  (  4) Values  : 0.540  0.000000  0.000000  0.047682    0.370
            Sigmas  :                             0.000050    0.031
            Shft/esd:                                0.17     0.76
 Fe2      moved  0.00A     sum(shift/e.s.d)**2 :    0.61

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 SC+3  (  5) Values  : 0.540  0.000000  0.000000  0.257903    0.521
            Sigmas  :                                       0.035
            Shft/esd:                                      -0.74
 Sc2      moved  0.00A     sum(shift/e.s.d)**2 :    0.55

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 1 :      2.38
 Calculated unit cell formula weight:   892.800, density:  4.513gm/cm**3

 Atom parameters for phase no. 2
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
                               Mx        My        Mz     |Moment|   Theta    Psi
 FE+3  (  1) Values  : 0.460  0.000000  0.000000  0.257890    0.521
            Sigmas  :                                       0.035
            Shft/esd:                                      -0.74

 FE+3  (  1) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.01
 FE1      moved  0.00A     sum(shift/e.s.d)**2 :    0.55

 FE+3  (  2) Values  : 0.460  0.666670  0.333330  0.591220    0.521
            Sigmas  :                                       0.035
            Shft/esd:                                      -0.74

 FE+3  (  2) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.01
 FE2      moved  0.00A     sum(shift/e.s.d)**2 :    0.55

 FE+3  (  3) Values  : 0.460  0.333330  0.666670  0.924560    0.521
            Sigmas  :                                       0.035
            Shft/esd:                                      -0.74

 FE+3  (  3) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.01
 FE3      moved  0.00A     sum(shift/e.s.d)**2 :    0.55

 FE+3  (  4) Values  : 0.460  0.000000  0.000000  0.757890    0.521
            Sigmas  :                                       0.035
            Shft/esd:                                      -0.74

 FE+3  (  4) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:           -0.01
 FE4      moved  0.00A     sum(shift/e.s.d)**2 :    0.55

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 FE+3  (  5) Values  : 0.460  0.666670  0.333330  0.091220    0.521
            Sigmas  :                                       0.035
            Shft/esd:                                      -0.74

 FE+3  (  5) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:           -0.01
 FE5      moved  0.00A     sum(shift/e.s.d)**2 :    0.55
```

```
 FE+3  (  6) Values  : 0.460  0.333330  0.666670  0.424560    0.521
              Sigmas  :                                      0.035
              Shft/esd:                                     -0.74

 FE+3  (  6) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:           -0.01
 FE6       moved  0.00A     sum(shift/e.s.d)**2 :    0.55

 FE+3  (  7) Values  : 0.540  0.000000  0.000000  0.047682    0.370
              Sigmas  :                             0.000050    0.031
              Shft/esd:                                0.17     0.76

 FE+3  (  7) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:           -0.01
 FE7       moved  0.00A     sum(shift/e.s.d)**2 :    0.61

 FE+3  (  8) Values  : 0.540  0.666670  0.333330  0.381012    0.370
              Sigmas  :                             0.000050    0.031
              Shft/esd:                                0.17     0.76

 FE+3  (  8) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:           -0.01
 FE8       moved  0.00A     sum(shift/e.s.d)**2 :    0.61

 FE+3  (  9) Values  : 0.540  0.333330  0.666670  0.714353    0.370
              Sigmas  :                             0.000050    0.031
              Shft/esd:                                0.17     0.76

 FE+3  (  9) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:           -0.01
 FE9       moved  0.00A     sum(shift/e.s.d)**2 :    0.61

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 FE+3  ( 10) Values  : 0.540  0.000000  0.000000  0.547683    0.370
              Sigmas  :                             0.000050    0.031
              Shft/esd:                                0.17     0.76

 FE+3  ( 10) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.01
 FE10      moved  0.00A     sum(shift/e.s.d)**2 :    0.61

 FE+3  ( 11) Values  : 0.540  0.666670  0.333330  0.881013    0.370
              Sigmas  :                             0.000050    0.031
              Shft/esd:                                0.17     0.76

 FE+3  ( 11) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.01
 FE11      moved  0.00A     sum(shift/e.s.d)**2 :    0.61

 FE+3  ( 12) Values  : 0.540  0.333330  0.666670  0.214353    0.370
              Sigmas  :                             0.000050    0.031
              Shft/esd:                                0.17     0.76

 FE+3  ( 12) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.01
 FE12      moved  0.00A     sum(shift/e.s.d)**2 :    0.61

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 2 :      7.00
 Calculated unit cell formula weight:   335.082, density:  1.694gm/cm**3

 Histogram scale factors:

 Histogram:    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 Scale    :    8.77103        8.77826        10.0709        0.00000        0.00000
 Sigmas   :   0.332558E-01   0.301481E-01   0.363082E-01    0.00000        0.00000
```

```
 Shift/esd:      -0.08          -0.11          -0.06           0.00           0.00
 Histogram scale factor sum(shift/error)**2 :      0.02

 Lattice parameters for powder data:
 Phase  1
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202475  5.202475 14.014487    90.000    90.000   120.000     328.494
 Sigmas   :  0.000004  0.000004  0.000113     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Phase  2
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202432  5.202446 14.014498    90.000    90.000   119.999     328.494
 Sigmas   :  0.000007  0.000007  0.000113     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Recprocal metric tensor sum(shift/error)**2 :      0.00
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 Diffractometer coefficients for powder data:
 Histogram :    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 C/L1/R/2Th:    4569.20        6162.13        2139.59        0.00000        0.00000
 Sigmas    :   0.105493        0.00000       0.153615        0.00000        0.00000
 Shift/esd :       0.00           0.00           0.00           0.00           0.00
 Dif A/Pola:  -0.969864       -2.51000        1.29554        0.00000        0.00000
 Sigmas    :   0.627692E-01    0.00000       0.698659E-01    0.00000        0.00000
 Shift/esd :       0.00           0.00           0.00           0.00           0.00
 Zero      :    1.90000        3.85000        9.03000        0.00000        0.00000
 Sigmas    :    0.00000        0.00000        0.00000        0.00000        0.00000
 Shift/esd :       0.00           0.00           0.00           0.00           0.00
 Dif. Cons. Sum(shift/error)**2 :      0.00

 Profile coefficients for histogram no.  1 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.512E-01                        1.560E-01
 Shift/esd:                                                   0.01                            -0.01
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.539E-02  1.628E+00
0.000E+00
 Sigmas   :                                              7.581E-01                        1.182E-01
 Shift/esd:                                                   0.01                            -0.01
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.469E-01
 Shift/esd:                                                   0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
```

```
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
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 Profile coefficients for histogram no.  1 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
0.000E+00
 Sigmas   :                                             8.512E-01                        1.560E-01
 Shift/esd:                                                  0.01                            -0.01
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.539E-02  1.628E+00
0.000E+00
 Sigmas   :                                             7.581E-01                        1.182E-01
 Shift/esd:                                                  0.01                            -0.01
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                             8.469E-01
 Shift/esd:                                                  0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
 Profile coef. sum(shift/error)**2 :      0.00

 Background coefficients for histogram no.  1:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   3.304273E-01  -1.784530E-02   5.279630E-02  -1.856671E-02  -9.806596E-03  -3.960142E-02
 Sigmas   :   4.614073E-03   8.661762E-03   7.904069E-03   7.311771E-03   6.852678E-03   6.160627E-03
 Shift/esd:           0.01           0.00          0.01           0.00           0.01           0.00
 Param.   :           7             8             9
 Coeff.   :  -1.851426E-02  -1.532087E-02  -7.128948E-03
 Sigmas   :   5.222123E-03   3.640635E-03   1.897181E-03
```

```
 Shift/esd:           0.01           0.00           0.01
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 Background coefficients for histogram no.  2:
 Param.   :           1              2              3              4              5              6
 Coeff.   :   2.736696E-01  -9.806543E-02   9.508059E-03  -1.771441E-02   1.125797E-02  -8.162072E-03
 Sigmas   :   2.500357E-03   4.625536E-03   4.215916E-03   3.985978E-03   3.837809E-03   3.726864E-03
 Shift/esd:           0.01           0.00           0.01           0.00           0.01           0.00
 Param.   :           7              8              9             10             11             12
 Coeff.   :   1.522888E-04  -1.499535E-02  -7.019843E-03   1.833594E-03   3.546810E-03  -1.694909E-02
 Sigmas   :   3.603216E-03   3.500137E-03   3.258566E-03   2.870752E-03   2.146390E-03   1.152073E-03
 Shift/esd:           0.01           0.01           0.01           0.02           0.02           0.05
 Background coef. sum(shift/error)**2 :      0.00

 CPU times for matrix build     1.73 sec; matrix inversion     0.00 sec
 Final variable sum((shift/esd)**2) for cycle1158:       1.24 Time:    1.73 sec
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 Restraint data statistics:
 No restraints used

 Powder data statistics                Fitted         -Bknd          pFree                  Average
              Bank Ndata Sum(w*d**2)  wRp     Rp    wRp     Rp    wRp     Rp  Npfree  DWd  Integral
 Hstgm  1 PNT   1  4524  4593.1     0.0694 0.1159 3.0076 0.6137 0.0000 0.0000     0   0.658   0.982
 Hstgm  2 PNT   2  3753  4940.9     0.0449 0.0945 0.1091 0.1134 0.0000 0.0000     0   0.462   0.990
 Hstgm  3 PNT   3  4808  4302.7     0.1278 0.1742 3.2083 0.7146 0.0000 0.0000     0   0.733   0.997
 Powder totals    13085  13837.     0.0614 0.1236 1.9004 0.4462 0.0000 0.0000     0   0.611

 No serial correlation in fit at 90% confidence for 1.952 < DWd < 2.048
 Cycle1159 There were  13085 observations.
 Total before-cycle CHI**2 (offset/sig) = 1.3837E+04 ( 4.9204E+00)
 Reduced CHI**2 =  1.061     for   43 variables

 Reflection data statistics
 Histogram  1  Type PNT   Nobs = 1302 R(F**2) =  0.1149
 Histogram  2  Type PNT   Nobs = 1071 R(F**2) =  0.0982
 Histogram  3  Type PNT   Nobs =  857 R(F**2) =  0.0805
 After matrix normalization and Marquardt modification:

    1 Columns of the    43 Column matrix are 0.0
 Full matrix recip. condition value & -log10 =   0.2037E-03      3.69
         Variable NoVarabl was not refined

 The value of the determinant is  1.2670*10.0**(   -22)

 Atom parameters for phase no. 1
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
 SC+3  (  1) Values  : 0.460  0.000000  0.000000  0.047676    0.354
             Sigmas  :                             0.000050    0.032
             Shft/esd:                               -0.11    -0.52
 Sc1       moved  0.00A     sum(shift/e.s.d)**2 :    0.28

 FE+3  (  2) Values  : 0.460  0.000000  0.000000  0.257903    0.540
             Sigmas  :                                       0.036
             Shft/esd:                                        0.53
 Fe1       moved  0.00A     sum(shift/e.s.d)**2 :    0.28

 O     (  3) Values  : 1.000  0.342323 -0.026074  0.817590    0.486
             Sigmas  :        0.000388  0.000227  0.000226    0.010
             Shft/esd:          -0.03     -0.02      0.15     0.10
 O1        moved  0.00A     sum(shift/e.s.d)**2 :    0.03

 FE+3  (  4) Values  : 0.540  0.000000  0.000000  0.047676    0.354
             Sigmas  :                             0.000050    0.032
             Shft/esd:                               -0.11    -0.52
 Fe2       moved  0.00A     sum(shift/e.s.d)**2 :    0.28

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 SC+3  (  5) Values  : 0.540  0.000000  0.000000  0.257903    0.540
```

```
            Sigmas  :                                        0.036
            Shft/esd:                                         0.53
 Sc2      moved  0.00A     sum(shift/e.s.d)**2 :    0.28

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 1 :      1.16
 Calculated unit cell formula weight:   892.800, density:  4.513gm/cm**3

 Atom parameters for phase no. 2
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
                                Mx        My        Mz     |Moment|   Theta    Psi
 FE+3  (  1) Values  : 0.460  0.000000  0.000000  0.257890    0.540
            Sigmas  :                                        0.036
            Shft/esd:                                         0.53

 FE+3  (  1) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE1      moved  0.00A     sum(shift/e.s.d)**2 :    0.28

 FE+3  (  2) Values  : 0.460  0.666670  0.333330  0.591220    0.540
            Sigmas  :                                        0.036
            Shft/esd:                                         0.53

 FE+3  (  2) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE2      moved  0.00A     sum(shift/e.s.d)**2 :    0.28

 FE+3  (  3) Values  : 0.460  0.333330  0.666670  0.924560    0.540
            Sigmas  :                                        0.036
            Shft/esd:                                         0.53

 FE+3  (  3) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE3      moved  0.00A     sum(shift/e.s.d)**2 :    0.28

 FE+3  (  4) Values  : 0.460  0.000000  0.000000  0.757890    0.540
            Sigmas  :                                        0.036
            Shft/esd:                                         0.53

 FE+3  (  4) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE4      moved  0.00A     sum(shift/e.s.d)**2 :    0.28

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 FE+3  (  5) Values  : 0.460  0.666670  0.333330  0.091220    0.540
            Sigmas  :                                        0.036
            Shft/esd:                                         0.53

 FE+3  (  5) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE5      moved  0.00A     sum(shift/e.s.d)**2 :    0.28

 FE+3  (  6) Values  : 0.460  0.333330  0.666670  0.424560    0.540
            Sigmas  :                                        0.036
            Shft/esd:                                         0.53

 FE+3  (  6) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE6      moved  0.00A     sum(shift/e.s.d)**2 :    0.28

 FE+3  (  7) Values  : 0.540  0.000000  0.000000  0.047676    0.354
            Sigmas  :                              0.000050    0.032
            Shft/esd:                                -0.11    -0.52

 FE+3  (  7) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
```

```
 FE7      moved  0.00A     sum(shift/e.s.d)**2 :    0.28

 FE+3  (  8) Values  : 0.540  0.666670  0.333330  0.381006    0.354
             Sigmas  :                             0.000050    0.032
             Shft/esd:                                -0.11    -0.52

 FE+3  (  8) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                         0.043    0.000    0.000
             Shft/esd:            0.00
 FE8      moved  0.00A     sum(shift/e.s.d)**2 :    0.28

 FE+3  (  9) Values  : 0.540  0.333330  0.666670  0.714347    0.354
             Sigmas  :                             0.000050    0.032
             Shft/esd:                                -0.11    -0.52

 FE+3  (  9) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                         0.043    0.000    0.000
             Shft/esd:            0.00
 FE9      moved  0.00A     sum(shift/e.s.d)**2 :    0.28

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 FE+3  ( 10) Values  : 0.540  0.000000  0.000000  0.547677    0.354
             Sigmas  :                             0.000050    0.032
             Shft/esd:                                -0.11    -0.52

 FE+3  ( 10) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                         0.043    0.000    0.000
             Shft/esd:            0.00
 FE10     moved  0.00A     sum(shift/e.s.d)**2 :    0.28

 FE+3  ( 11) Values  : 0.540  0.666670  0.333330  0.881007    0.354
             Sigmas  :                             0.000050    0.032
             Shft/esd:                                -0.11    -0.52

 FE+3  ( 11) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                         0.043    0.000    0.000
             Shft/esd:            0.00
 FE11     moved  0.00A     sum(shift/e.s.d)**2 :    0.28

 FE+3  ( 12) Values  : 0.540  0.333330  0.666670  0.214347    0.354
             Sigmas  :                             0.000050    0.032
             Shft/esd:                                -0.11    -0.52

 FE+3  ( 12) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                         0.043    0.000    0.000
             Shft/esd:            0.00
 FE12     moved  0.00A     sum(shift/e.s.d)**2 :    0.28

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 2 :      3.38
 Calculated unit cell formula weight:   335.082, density:  1.694gm/cm**3

 Histogram scale factors:

 Histogram:    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 Scale    :    8.77307        8.78074        10.0725        0.00000        0.00000
 Sigmas   :   0.331547E-01   0.299920E-01   0.362525E-01    0.00000        0.00000
 Shift/esd:       0.06           0.08           0.05           0.00           0.00
 Histogram scale factor sum(shift/error)**2 :      0.01

 Lattice parameters for powder data:
 Phase  1
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202475  5.202475 14.014489    90.000    90.000   120.000     328.494
 Sigmas   :  0.000004  0.000004  0.000113     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Phase  2
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202432  5.202446 14.014500    90.000    90.000   119.999     328.494
 Sigmas   :  0.000007  0.000007  0.000113     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Recprocal metric tensor sum(shift/error)**2 :      0.00
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```

```
 Diffractometer coefficients for powder data:
 Histogram :    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 C/L1/R/2Th:    4569.20        6162.13        2139.59        0.00000        0.00000
 Sigmas    :   0.105498        0.00000       0.153598        0.00000        0.00000
 Shift/esd :       0.01           0.00           0.00           0.00           0.00
 Dif A/Pola:  -0.970344       -2.51000        1.29547        0.00000        0.00000
 Sigmas    :   0.627769E-01    0.00000       0.698622E-01    0.00000        0.00000
 Shift/esd :       0.01           0.00           0.00           0.00           0.00
 Zero      :    1.90000        3.85000        9.03000        0.00000        0.00000
 Sigmas    :    0.00000        0.00000        0.00000        0.00000        0.00000
 Shift/esd :       0.01           0.00           0.00           0.00           0.00
 Dif. Cons. Sum(shift/error)**2 :      0.00

 Profile coefficients for histogram no.  1 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.515E-01                        1.561E-01
 Shift/esd:                                                   0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.532E-02  1.628E+00
0.000E+00
 Sigmas   :                                              7.583E-01                        1.182E-01
 Shift/esd:                                                   0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.469E-01
 Shift/esd:                                                   0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
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 Profile coefficients for histogram no.  1 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
```

```
0.000E+00
 Sigmas   :                                              8.515E-01                        1.561E-01
 Shift/esd:                                                   0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.532E-02  1.628E+00
0.000E+00
 Sigmas   :                                              7.583E-01                        1.182E-01
 Shift/esd:                                                   0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.469E-01
 Shift/esd:                                                   0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
 Profile coef. sum(shift/error)**2 :      0.00

 Background coefficients for histogram no.  1:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   3.303997E-01  -1.781429E-02   5.273131E-02  -1.853438E-02  -9.865087E-03  -3.958838E-02
 Sigmas   :   4.613976E-03   8.661765E-03   7.903889E-03   7.311775E-03   6.852463E-03   6.160628E-03
 Shift/esd:          -0.01           0.00          -0.01           0.00          -0.01           0.00
 Param.   :           7             8             9
 Coeff.   :  -1.857017E-02  -1.532964E-02  -7.150317E-03
 Sigmas   :   5.221894E-03   3.640648E-03   1.897035E-03
 Shift/esd:          -0.01           0.00          -0.01
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 Background coefficients for histogram no.  2:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   2.736521E-01  -9.805740E-02   9.465559E-03  -1.770812E-02   1.122679E-02  -8.160715E-03
 Sigmas   :   2.500101E-03   4.625359E-03   4.215546E-03   3.985877E-03   3.837598E-03   3.726889E-03
 Shift/esd:          -0.01           0.00          -0.01           0.00          -0.01           0.00
 Param.   :           7             8             9            10            11            12
 Coeff.   :   1.290782E-04  -1.502829E-02  -7.053775E-03   1.797236E-03   3.511501E-03  -1.699015E-02
 Sigmas   :   3.603122E-03   3.500125E-03   3.258444E-03   2.870640E-03   2.146235E-03   1.151758E-03
 Shift/esd:          -0.01          -0.01          -0.01          -0.01          -0.02          -0.04
 Background coef. sum(shift/error)**2 :      0.00

 CPU times for matrix build     1.64 sec; matrix inversion     0.02 sec
```

```
 Final variable sum((shift/esd)**2) for cycle1159:       0.61 Time:    1.66 sec
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 Restraint data statistics:
 No restraints used

 Powder data statistics                Fitted         -Bknd          pFree                 Average
             Bank Ndata Sum(w*d**2)  wRp     Rp    wRp     Rp    wRp     Rp  Npfree  DWd  Integral
 Hstgm  1 PNT   1  4524  4592.5     0.0694 0.1159 3.0072 0.6136 0.0000 0.0000     0   0.658   0.982
 Hstgm  2 PNT   2  3753  4940.7     0.0449 0.0945 0.1091 0.1135 0.0000 0.0000     0   0.462   0.990
 Hstgm  3 PNT   3  4808  4303.2     0.1278 0.1742 3.2083 0.7146 0.0000 0.0000     0   0.732   0.997
 Powder totals    13085  13836.     0.0614 0.1237 1.9002 0.4462 0.0000 0.0000     0   0.611

 No serial correlation in fit at 90% confidence for 1.952 < DWd < 2.048
 Cycle1160 There were  13085 observations.
 Total before-cycle CHI**2 (offset/sig) = 1.3836E+04 ( 4.9191E+00)
 Reduced CHI**2 =  1.061     for   43 variables

 Reflection data statistics
 Histogram  1  Type PNT   Nobs = 1302 R(F**2) =  0.1149
 Histogram  2  Type PNT   Nobs = 1071 R(F**2) =  0.0982
 Histogram  3  Type PNT   Nobs =  857 R(F**2) =  0.0805
 After matrix normalization and Marquardt modification:

    1 Columns of the    43 Column matrix are 0.0
 Full matrix recip. condition value & -log10 =   0.2034E-03      3.69
         Variable NoVarabl was not refined

 The value of the determinant is  1.3134*10.0**(   -22)

 Atom parameters for phase no. 1
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
 SC+3  (  1) Values  : 0.460  0.000000  0.000000  0.047681    0.366
             Sigmas  :                             0.000050    0.031
             Shft/esd:                                0.09     0.40
 Sc1      moved  0.00A     sum(shift/e.s.d)**2 :    0.17

 FE+3  (  2) Values  : 0.460  0.000000  0.000000  0.257903    0.526
             Sigmas  :                                        0.035
             Shft/esd:                                       -0.39
 Fe1      moved  0.00A     sum(shift/e.s.d)**2 :    0.16

 O     (  3) Values  : 1.000  0.342328 -0.026072  0.817567    0.486
             Sigmas  :        0.000390  0.000228  0.000227    0.010
             Shft/esd:           0.01      0.01     -0.11    -0.06
 O1       moved  0.00A     sum(shift/e.s.d)**2 :    0.02

 FE+3  (  4) Values  : 0.540  0.000000  0.000000  0.047681    0.366
             Sigmas  :                             0.000050    0.031
             Shft/esd:                                0.09     0.40
 Fe2      moved  0.00A     sum(shift/e.s.d)**2 :    0.17

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 SC+3  (  5) Values  : 0.540  0.000000  0.000000  0.257903    0.526
             Sigmas  :                                        0.035
             Shft/esd:                                       -0.39
 Sc2      moved  0.00A     sum(shift/e.s.d)**2 :    0.16

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 1 :      0.66
 Calculated unit cell formula weight:   892.800, density:  4.513gm/cm**3

 Atom parameters for phase no. 2
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
                                 Mx        My        Mz     |Moment|   Theta    Psi
 FE+3  (  1) Values  : 0.460  0.000000  0.000000  0.257890    0.526
             Sigmas  :                                        0.035
             Shft/esd:                                       -0.39

 FE+3  (  1) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
```

```
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE1      moved  0.00A     sum(shift/e.s.d)**2 :    0.16

 FE+3  (  2) Values  : 0.460  0.666670  0.333330  0.591220    0.526
            Sigmas  :                                       0.035
            Shft/esd:                                       -0.39

 FE+3  (  2) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE2      moved  0.00A     sum(shift/e.s.d)**2 :    0.16

 FE+3  (  3) Values  : 0.460  0.333330  0.666670  0.924560    0.526
            Sigmas  :                                       0.035
            Shft/esd:                                       -0.39

 FE+3  (  3) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE3      moved  0.00A     sum(shift/e.s.d)**2 :    0.16

 FE+3  (  4) Values  : 0.460  0.000000  0.000000  0.757890    0.526
            Sigmas  :                                       0.035
            Shft/esd:                                       -0.39

 FE+3  (  4) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE4      moved  0.00A     sum(shift/e.s.d)**2 :    0.16

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 FE+3  (  5) Values  : 0.460  0.666670  0.333330  0.091220    0.526
            Sigmas  :                                       0.035
            Shft/esd:                                       -0.39

 FE+3  (  5) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE5      moved  0.00A     sum(shift/e.s.d)**2 :    0.16

 FE+3  (  6) Values  : 0.460  0.333330  0.666670  0.424560    0.526
            Sigmas  :                                       0.035
            Shft/esd:                                       -0.39

 FE+3  (  6) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE6      moved  0.00A     sum(shift/e.s.d)**2 :    0.16

 FE+3  (  7) Values  : 0.540  0.000000  0.000000  0.047681    0.366
            Sigmas  :                               0.000050    0.031
            Shft/esd:                                   0.09     0.40

 FE+3  (  7) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE7      moved  0.00A     sum(shift/e.s.d)**2 :    0.17

 FE+3  (  8) Values  : 0.540  0.666670  0.333330  0.381011    0.366
            Sigmas  :                               0.000050    0.031
            Shft/esd:                                   0.09     0.40

 FE+3  (  8) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE8      moved  0.00A     sum(shift/e.s.d)**2 :    0.17

 FE+3  (  9) Values  : 0.540  0.333330  0.666670  0.714352    0.366
            Sigmas  :                               0.000050    0.031
            Shft/esd:                                   0.09     0.40

 FE+3  (  9) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
```

```
            Shft/esd:            0.00
 FE9      moved  0.00A     sum(shift/e.s.d)**2 :    0.17

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 FE+3  ( 10) Values  : 0.540  0.000000  0.000000  0.547682    0.366
             Sigmas  :                             0.000050    0.031
             Shft/esd:                                0.09     0.40

 FE+3  ( 10) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE10     moved  0.00A     sum(shift/e.s.d)**2 :    0.17

 FE+3  ( 11) Values  : 0.540  0.666670  0.333330  0.881012    0.366
             Sigmas  :                             0.000050    0.031
             Shft/esd:                                0.09     0.40

 FE+3  ( 11) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE11     moved  0.00A     sum(shift/e.s.d)**2 :    0.17

 FE+3  ( 12) Values  : 0.540  0.333330  0.666670  0.214352    0.366
             Sigmas  :                             0.000050    0.031
             Shft/esd:                                0.09     0.40

 FE+3  ( 12) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE12     moved  0.00A     sum(shift/e.s.d)**2 :    0.17

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 2 :      1.94
 Calculated unit cell formula weight:   335.082, density:  1.694gm/cm**3

 Histogram scale factors:

 Histogram:    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 Scale    :    8.77175        8.77910        10.0715        0.00000        0.00000
 Sigmas   :   0.332279E-01   0.301041E-01   0.362925E-01    0.00000        0.00000
 Shift/esd:      -0.04          -0.05          -0.03           0.00           0.00
 Histogram scale factor sum(shift/error)**2 :      0.01

 Lattice parameters for powder data:
 Phase  1
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202475  5.202475 14.014489    90.000    90.000   120.000     328.494
 Sigmas   :  0.000004  0.000004  0.000114     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Phase  2
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202432  5.202446 14.014500    90.000    90.000   119.999     328.494
 Sigmas   :  0.000007  0.000007  0.000114     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Recprocal metric tensor sum(shift/error)**2 :      0.00
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 Diffractometer coefficients for powder data:
 Histogram :    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 C/L1/R/2Th:    4569.20        6162.13        2139.59        0.00000        0.00000
 Sigmas    :   0.105498        0.00000       0.153608        0.00000        0.00000
 Shift/esd :      -0.01           0.00           0.00           0.00           0.00
 Dif A/Pola:  -0.969971       -2.51000        1.29553        0.00000        0.00000
 Sigmas    :   0.627730E-01    0.00000       0.698632E-01    0.00000        0.00000
 Shift/esd :      -0.01           0.00           0.00           0.00           0.00
 Zero      :    1.90000        3.85000        9.03000        0.00000        0.00000
 Sigmas    :    0.00000        0.00000        0.00000        0.00000        0.00000
 Shift/esd :      -0.01           0.00           0.00           0.00           0.00
 Dif. Cons. Sum(shift/error)**2 :      0.00

 Profile coefficients for histogram no.  1 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
```

```
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.514E-01                        1.560E-01
 Shift/esd:                                                  0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.552E-02  1.628E+00
0.000E+00
 Sigmas   :                                              7.582E-01                        1.182E-01
 Shift/esd:                                                  0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.469E-01
 Shift/esd:                                                  0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
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 Profile coefficients for histogram no.  1 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.514E-01                        1.560E-01
 Shift/esd:                                                  0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
```

```
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.552E-02  1.628E+00
0.000E+00
 Sigmas   :                                              7.582E-01                       1.182E-01
 Shift/esd:                                                   0.00                            0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.469E-01
 Shift/esd:                                                   0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
 Profile coef. sum(shift/error)**2 :      0.00

 Background coefficients for histogram no.  1:
 Param.   :           1              2              3              4              5              6
 Coeff.   :   3.304170E-01  -1.783141E-02   5.277473E-02  -1.855332E-02  -9.825979E-03  -3.959480E-02
 Sigmas   :   4.614030E-03   8.661701E-03   7.903991E-03   7.311732E-03   6.852592E-03   6.160592E-03
 Shift/esd:           0.00           0.00           0.01           0.00           0.01           0.00
 Param.   :           7              8              9
 Coeff.   :  -1.853162E-02  -1.532236E-02  -7.136061E-03
 Sigmas   :   5.222030E-03   3.640612E-03   1.897122E-03
 Shift/esd:           0.01           0.00           0.01
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 Background coefficients for histogram no.  2:
 Param.   :           1              2              3              4              5              6
 Coeff.   :   2.736629E-01  -9.805943E-02   9.493842E-03  -1.770923E-02   1.124730E-02  -8.159869E-03
 Sigmas   :   2.500264E-03   4.625425E-03   4.215795E-03   3.985913E-03   3.837736E-03   3.726856E-03
 Shift/esd:           0.00           0.00           0.01           0.00           0.01           0.00
 Param.   :           7              8              9             10             11             12
 Coeff.   :   1.446880E-04  -1.500416E-02  -7.029905E-03   1.823175E-03   3.536572E-03  -1.696094E-02
 Sigmas   :   3.603180E-03   3.500121E-03   3.258511E-03   2.870693E-03   2.146326E-03   1.151982E-03
 Shift/esd:           0.00           0.01           0.01           0.01           0.01           0.03
 Background coef. sum(shift/error)**2 :      0.00

 CPU times for matrix build     1.59 sec; matrix inversion     0.00 sec
 Final variable sum((shift/esd)**2) for cycle1160:       0.35 Time:    1.59 sec
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 Restraint data statistics:
 No restraints used

 Powder data statistics                Fitted         -Bknd          pFree                 Average
              Bank Ndata Sum(w*d**2)  wRp     Rp    wRp     Rp    wRp     Rp  Npfree  DWd  Integral
 Hstgm  1 PNT   1  4524  4592.8     0.0694 0.1159 3.0075 0.6137 0.0000 0.0000     0   0.658   0.982
 Hstgm  2 PNT   2  3753  4940.9     0.0449 0.0945 0.1091 0.1135 0.0000 0.0000     0   0.462   0.990
 Hstgm  3 PNT   3  4808  4302.8     0.1278 0.1742 3.2083 0.7146 0.0000 0.0000     0   0.733   0.997
 Powder totals    13085  13836.     0.0614 0.1237 1.9004 0.4462 0.0000 0.0000     0   0.611

 No serial correlation in fit at 90% confidence for 1.952 < DWd < 2.048
 Cycle1161 There were  13085 observations.
```

```
 Total before-cycle CHI**2 (offset/sig) = 1.3836E+04 ( 4.9191E+00)
 Reduced CHI**2 =  1.061     for   43 variables

 Reflection data statistics
 Histogram  1  Type PNT   Nobs = 1302 R(F**2) =  0.1148
 Histogram  2  Type PNT   Nobs = 1071 R(F**2) =  0.0982
 Histogram  3  Type PNT   Nobs =  857 R(F**2) =  0.0805
 After matrix normalization and Marquardt modification:

    1 Columns of the    43 Column matrix are 0.0
 Full matrix recip. condition value & -log10 =   0.2036E-03      3.69
        Variable NoVarabl was not refined

 The value of the determinant is  1.2766*10.0**(   -22)

 Atom parameters for phase no. 1
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
 SC+3  (  1) Values  : 0.460  0.000000  0.000000  0.047678    0.357
             Sigmas  :                             0.000050    0.032
             Shft/esd:                                -0.06    -0.28
 Sc1      moved  0.00A     sum(shift/e.s.d)**2 :    0.08

 FE+3  (  2) Values  : 0.460  0.000000  0.000000  0.257903    0.537
             Sigmas  :                                       0.036
             Shft/esd:                                        0.29
 Fe1      moved  0.00A     sum(shift/e.s.d)**2 :    0.08

 O     (  3) Values  : 1.000  0.342323 -0.026074  0.817584    0.486
             Sigmas  :        0.000389  0.000227  0.000226    0.010
             Shft/esd:           -0.01     -0.01      0.08     0.05
 O1       moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  4) Values  : 0.540  0.000000  0.000000  0.047678    0.357
             Sigmas  :                             0.000050    0.032
             Shft/esd:                                -0.06    -0.28
 Fe2      moved  0.00A     sum(shift/e.s.d)**2 :    0.08

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 SC+3  (  5) Values  : 0.540  0.000000  0.000000  0.257903    0.537
             Sigmas  :                                       0.036
             Shft/esd:                                        0.29
 Sc2      moved  0.00A     sum(shift/e.s.d)**2 :    0.08

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 1 :      0.34
 Calculated unit cell formula weight:   892.800, density:  4.513gm/cm**3

 Atom parameters for phase no. 2
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
                               Mx        My        Mz     |Moment|   Theta    Psi
 FE+3  (  1) Values  : 0.460  0.000000  0.000000  0.257890    0.537
             Sigmas  :                                       0.036
             Shft/esd:                                        0.29

 FE+3  (  1) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE1      moved  0.00A     sum(shift/e.s.d)**2 :    0.08

 FE+3  (  2) Values  : 0.460  0.666670  0.333330  0.591220    0.537
             Sigmas  :                                       0.036
             Shft/esd:                                        0.29

 FE+3  (  2) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE2      moved  0.00A     sum(shift/e.s.d)**2 :    0.08

 FE+3  (  3) Values  : 0.460  0.333330  0.666670  0.924560    0.537
             Sigmas  :                                       0.036
             Shft/esd:                                        0.29
```

```
 FE+3  (  3) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE3      moved  0.00A     sum(shift/e.s.d)**2 :    0.08

 FE+3  (  4) Values  : 0.460  0.000000  0.000000  0.757890    0.537
            Sigmas  :                                       0.036
            Shft/esd:                                        0.29

 FE+3  (  4) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE4      moved  0.00A     sum(shift/e.s.d)**2 :    0.08

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 FE+3  (  5) Values  : 0.460  0.666670  0.333330  0.091220    0.537
            Sigmas  :                                       0.036
            Shft/esd:                                        0.29

 FE+3  (  5) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE5      moved  0.00A     sum(shift/e.s.d)**2 :    0.08

 FE+3  (  6) Values  : 0.460  0.333330  0.666670  0.424560    0.537
            Sigmas  :                                       0.036
            Shft/esd:                                        0.29

 FE+3  (  6) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE6      moved  0.00A     sum(shift/e.s.d)**2 :    0.08

 FE+3  (  7) Values  : 0.540  0.000000  0.000000  0.047678    0.357
            Sigmas  :                               0.000050    0.032
            Shft/esd:                                  -0.06    -0.28

 FE+3  (  7) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE7      moved  0.00A     sum(shift/e.s.d)**2 :    0.08

 FE+3  (  8) Values  : 0.540  0.666670  0.333330  0.381008    0.357
            Sigmas  :                               0.000050    0.032
            Shft/esd:                                  -0.06    -0.28

 FE+3  (  8) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE8      moved  0.00A     sum(shift/e.s.d)**2 :    0.08

 FE+3  (  9) Values  : 0.540  0.333330  0.666670  0.714349    0.357
            Sigmas  :                               0.000050    0.032
            Shft/esd:                                  -0.06    -0.28

 FE+3  (  9) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE9      moved  0.00A     sum(shift/e.s.d)**2 :    0.08

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 FE+3  ( 10) Values  : 0.540  0.000000  0.000000  0.547679    0.357
            Sigmas  :                               0.000050    0.032
            Shft/esd:                                  -0.06    -0.28

 FE+3  ( 10) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE10     moved  0.00A     sum(shift/e.s.d)**2 :    0.08

 FE+3  ( 11) Values  : 0.540  0.666670  0.333330  0.881009    0.357
            Sigmas  :                               0.000050    0.032
```

```
            Shft/esd:                                -0.06    -0.28

 FE+3  ( 11) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                         0.043    0.000    0.000
            Shft/esd:            0.00
 FE11     moved  0.00A     sum(shift/e.s.d)**2 :    0.08

 FE+3  ( 12) Values  : 0.540  0.333330  0.666670  0.214349    0.357
            Sigmas  :                            0.000050    0.032
            Shft/esd:                               -0.06    -0.28

 FE+3  ( 12) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                         0.043    0.000    0.000
            Shft/esd:            0.00
 FE12     moved  0.00A     sum(shift/e.s.d)**2 :    0.08

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 2 :      1.00
 Calculated unit cell formula weight:   335.082, density:  1.694gm/cm**3

 Histogram scale factors:

 Histogram:    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 Scale    :    8.77281        8.78039        10.0723        0.00000        0.00000
 Sigmas   :   0.331739E-01   0.300214E-01   0.362630E-01    0.00000        0.00000
 Shift/esd:       0.03           0.04           0.02           0.00           0.00
 Histogram scale factor sum(shift/error)**2 :      0.00

 Lattice parameters for powder data:
 Phase  1
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202475  5.202475 14.014489    90.000    90.000   120.000     328.494
 Sigmas   :  0.000004  0.000004  0.000114     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Phase  2
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202432  5.202446 14.014500    90.000    90.000   119.999     328.494
 Sigmas   :  0.000007  0.000007  0.000114     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Recprocal metric tensor sum(shift/error)**2 :      0.00
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 Diffractometer coefficients for powder data:
 Histogram :    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 C/L1/R/2Th:    4569.20        6162.13        2139.59        0.00000        0.00000
 Sigmas    :   0.105502        0.00000       0.153601        0.00000        0.00000
 Shift/esd :       0.00           0.00           0.00           0.00           0.00
 Dif A/Pola:  -0.970269       -2.51000        1.29550        0.00000        0.00000
 Sigmas    :   0.627774E-01    0.00000       0.698621E-01    0.00000        0.00000
 Shift/esd :       0.00           0.00           0.00           0.00           0.00
 Zero      :    1.90000        3.85000        9.03000        0.00000        0.00000
 Sigmas    :    0.00000        0.00000        0.00000        0.00000        0.00000
 Shift/esd :       0.00           0.00           0.00           0.00           0.00
 Dif. Cons. Sum(shift/error)**2 :      0.00

 Profile coefficients for histogram no.  1 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.514E-01                        1.561E-01
 Shift/esd:                                                  0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  1:
```

```
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.543E-02  1.628E+00
0.000E+00
 Sigmas   :                                              7.583E-01                        1.182E-01
 Shift/esd:                                                  0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.469E-01
 Shift/esd:                                                  0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
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 Profile coefficients for histogram no.  1 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.514E-01                        1.561E-01
 Shift/esd:                                                  0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.543E-02  1.628E+00
0.000E+00
 Sigmas   :                                              7.583E-01                        1.182E-01
 Shift/esd:                                                  0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
```

```
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.469E-01
 Shift/esd:                                                   0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
 Profile coef. sum(shift/error)**2 :      0.00

 Background coefficients for histogram no.  1:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   3.304023E-01  -1.781683E-02   5.273972E-02  -1.853761E-02  -9.857190E-03  -3.958889E-02
 Sigmas   :   4.614026E-03   8.661845E-03   7.903988E-03   7.311811E-03   6.852502E-03   6.160600E-03
 Shift/esd:           0.00           0.00           0.00           0.00           0.00           0.00
 Param.   :           7             8             9
 Coeff.   :  -1.856144E-02  -1.532744E-02  -7.147302E-03
 Sigmas   :   5.221894E-03   3.640610E-03   1.897042E-03
 Shift/esd:          -0.01           0.00          -0.01
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 Background coefficients for histogram no.  2:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   2.736536E-01  -9.805645E-02   9.470975E-03  -1.770705E-02   1.123059E-02  -8.159879E-03
 Sigmas   :   2.500180E-03   4.625460E-03   4.215688E-03   3.985947E-03   3.837672E-03   3.726899E-03
 Shift/esd:           0.00           0.00          -0.01           0.00           0.00           0.00
 Param.   :           7             8             9            10            11            12
 Coeff.   :   1.322849E-04  -1.502200E-02  -7.048016E-03   1.803728E-03   3.517767E-03  -1.698280E-02
 Sigmas   :   3.603150E-03   3.500139E-03   3.258474E-03   2.870663E-03   2.146260E-03   1.151819E-03
 Shift/esd:           0.00          -0.01          -0.01          -0.01          -0.01          -0.02
 Background coef. sum(shift/error)**2 :      0.00

 CPU times for matrix build     1.66 sec; matrix inversion     0.03 sec
 Final variable sum((shift/esd)**2) for cycle1161:       0.18 Time:    1.69 sec
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 Restraint data statistics:
 No restraints used

 Powder data statistics                Fitted         -Bknd          pFree                  Average
              Bank Ndata Sum(w*d**2)  wRp     Rp    wRp     Rp    wRp     Rp  Npfree  DWd  Integral
 Hstgm  1 PNT   1  4524  4592.5     0.0694 0.1159 3.0072 0.6136 0.0000 0.0000     0   0.658   0.982
 Hstgm  2 PNT   2  3753  4940.8     0.0449 0.0945 0.1091 0.1135 0.0000 0.0000     0   0.462   0.990
 Hstgm  3 PNT   3  4808  4303.1     0.1278 0.1742 3.2083 0.7146 0.0000 0.0000     0   0.732   0.997
 Powder totals    13085  13836.     0.0614 0.1237 1.9002 0.4462 0.0000 0.0000     0   0.611

 No serial correlation in fit at 90% confidence for 1.952 < DWd < 2.048
 Cycle1162 There were  13085 observations.
 Total before-cycle CHI**2 (offset/sig) = 1.3836E+04 ( 4.9187E+00)
 Reduced CHI**2 =  1.061     for   43 variables

 Reflection data statistics
 Histogram  1  Type PNT   Nobs = 1302 R(F**2) =  0.1148
 Histogram  2  Type PNT   Nobs = 1071 R(F**2) =  0.0982
 Histogram  3  Type PNT   Nobs =  857 R(F**2) =  0.0805
 After matrix normalization and Marquardt modification:

    1 Columns of the    43 Column matrix are 0.0
 Full matrix recip. condition value & -log10 =   0.2035E-03      3.69
         Variable NoVarabl was not refined

 The value of the determinant is  1.3026*10.0**(   -22)

 Atom parameters for phase no. 1
                      frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
```

```
100*U23
 SC+3  (  1) Values  : 0.460  0.000000  0.000000  0.047680    0.364
            Sigmas  :                             0.000050    0.032
            Shft/esd:                                0.05     0.21
 Sc1      moved  0.00A     sum(shift/e.s.d)**2 :    0.05

 FE+3  (  2) Values  : 0.460  0.000000  0.000000  0.257903    0.529
            Sigmas  :                                        0.035
            Shft/esd:                                       -0.21
 Fe1      moved  0.00A     sum(shift/e.s.d)**2 :    0.05

 O     (  3) Values  : 1.000  0.342326 -0.026073  0.817571    0.486
            Sigmas  :        0.000389  0.000228  0.000227    0.010
            Shft/esd:           0.01      0.00     -0.06    -0.03
 O1       moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  4) Values  : 0.540  0.000000  0.000000  0.047680    0.364
            Sigmas  :                             0.000050    0.032
            Shft/esd:                                0.05     0.21
 Fe2      moved  0.00A     sum(shift/e.s.d)**2 :    0.05

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 SC+3  (  5) Values  : 0.540  0.000000  0.000000  0.257903    0.529
            Sigmas  :                                        0.035
            Shft/esd:                                       -0.21
 Sc2      moved  0.00A     sum(shift/e.s.d)**2 :    0.05

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 1 :      0.19
 Calculated unit cell formula weight:   892.800, density:  4.513gm/cm**3

 Atom parameters for phase no. 2
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
                               Mx        My        Mz     |Moment|   Theta    Psi
 FE+3  (  1) Values  : 0.460  0.000000  0.000000  0.257890    0.529
            Sigmas  :                                        0.035
            Shft/esd:                                       -0.21

 FE+3  (  1) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                         0.043    0.000    0.000
            Shft/esd:            0.00
 FE1      moved  0.00A     sum(shift/e.s.d)**2 :    0.05

 FE+3  (  2) Values  : 0.460  0.666670  0.333330  0.591220    0.529
            Sigmas  :                                        0.035
            Shft/esd:                                       -0.21

 FE+3  (  2) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                         0.043    0.000    0.000
            Shft/esd:            0.00
 FE2      moved  0.00A     sum(shift/e.s.d)**2 :    0.05

 FE+3  (  3) Values  : 0.460  0.333330  0.666670  0.924560    0.529
            Sigmas  :                                        0.035
            Shft/esd:                                       -0.21

 FE+3  (  3) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                         0.043    0.000    0.000
            Shft/esd:            0.00
 FE3      moved  0.00A     sum(shift/e.s.d)**2 :    0.05

 FE+3  (  4) Values  : 0.460  0.000000  0.000000  0.757890    0.529
            Sigmas  :                                        0.035
            Shft/esd:                                       -0.21

 FE+3  (  4) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                         0.043    0.000    0.000
            Shft/esd:            0.00
 FE4      moved  0.00A     sum(shift/e.s.d)**2 :    0.05

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```

```
 FE+3  (  5) Values  : 0.460  0.666670  0.333330  0.091220    0.529
             Sigmas  :                                      0.035
             Shft/esd:                                     -0.21

 FE+3  (  5) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                       0.043    0.000    0.000
             Shft/esd:            0.00
 FE5      moved  0.00A     sum(shift/e.s.d)**2 :    0.05

 FE+3  (  6) Values  : 0.460  0.333330  0.666670  0.424560    0.529
             Sigmas  :                                      0.035
             Shft/esd:                                     -0.21

 FE+3  (  6) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                       0.043    0.000    0.000
             Shft/esd:            0.00
 FE6      moved  0.00A     sum(shift/e.s.d)**2 :    0.05

 FE+3  (  7) Values  : 0.540  0.000000  0.000000  0.047680    0.364
             Sigmas  :                               0.000050    0.032
             Shft/esd:                                   0.05     0.21

 FE+3  (  7) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                       0.043    0.000    0.000
             Shft/esd:            0.00
 FE7      moved  0.00A     sum(shift/e.s.d)**2 :    0.05

 FE+3  (  8) Values  : 0.540  0.666670  0.333330  0.381010    0.364
             Sigmas  :                               0.000050    0.032
             Shft/esd:                                   0.05     0.21

 FE+3  (  8) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                       0.043    0.000    0.000
             Shft/esd:            0.00
 FE8      moved  0.00A     sum(shift/e.s.d)**2 :    0.05

 FE+3  (  9) Values  : 0.540  0.333330  0.666670  0.714351    0.364
             Sigmas  :                               0.000050    0.032
             Shft/esd:                                   0.05     0.21

 FE+3  (  9) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                       0.043    0.000    0.000
             Shft/esd:            0.00
 FE9      moved  0.00A     sum(shift/e.s.d)**2 :    0.05

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 FE+3  ( 10) Values  : 0.540  0.000000  0.000000  0.547681    0.364
             Sigmas  :                               0.000050    0.032
             Shft/esd:                                   0.05     0.21

 FE+3  ( 10) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                       0.043    0.000    0.000
             Shft/esd:            0.00
 FE10     moved  0.00A     sum(shift/e.s.d)**2 :    0.05

 FE+3  ( 11) Values  : 0.540  0.666670  0.333330  0.881011    0.364
             Sigmas  :                               0.000050    0.032
             Shft/esd:                                   0.05     0.21

 FE+3  ( 11) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                       0.043    0.000    0.000
             Shft/esd:            0.00
 FE11     moved  0.00A     sum(shift/e.s.d)**2 :    0.05

 FE+3  ( 12) Values  : 0.540  0.333330  0.666670  0.214351    0.364
             Sigmas  :                               0.000050    0.032
             Shft/esd:                                   0.05     0.21

 FE+3  ( 12) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                       0.043    0.000    0.000
             Shft/esd:            0.00
 FE12     moved  0.00A     sum(shift/e.s.d)**2 :    0.05

 Maximum atom shift:   0.00
```

Atomic parameter sum(shift/error)**2 for phase 2 :   0.56
Calculated unit cell formula weight: 335.082, density: 1.694gm/cm**3

Histogram scale factors:

Histogram:	1 PNT	2 PNT	3 PNT	4 PNT*	5 PXC*
Scale :	8.77207	8.77948	10.0717	0.00000	0.00000
Sigmas :	0.332132E-01	0.300817E-01	0.362845E-01	0.00000	0.00000
Shift/esd:	-0.02	-0.03	-0.02	0.00	0.00

Histogram scale factor sum(shift/error)**2 :   0.00

Lattice parameters for powder data:
Phase 1

	a	b	c	alpha	beta	gamma	volume
Value :	5.202475	5.202475	14.014489	90.000	90.000	120.000	328.494
Sigmas :	0.000004	0.000004	0.000114	0.000	0.000	0.000	0.003

Recprocal metric tensor shift factor = 100%
Phase 2

	a	b	c	alpha	beta	gamma	volume
Value :	5.202432	5.202446	14.014500	90.000	90.000	119.999	328.494
Sigmas :	0.000007	0.000007	0.000114	0.000	0.000	0.000	0.003

Recprocal metric tensor shift factor = 100%
Recprocal metric tensor sum(shift/error)**2 :   0.00

Diffractometer coefficients for powder data:

Histogram :	1 PNT	2 PNT	3 PNT	4 PNT*	5 PXC*
C/L1/R/2Th:	4569.20	6162.13	2139.59	0.00000	0.00000
Sigmas :	0.105499	0.00000	0.153605	0.00000	0.00000
Shift/esd :	0.00	0.00	0.00	0.00	0.00
Dif A/Pola:	-0.970085	-2.51000	1.29549	0.00000	0.00000
Sigmas :	0.627740E-01	0.00000	0.698624E-01	0.00000	0.00000
Shift/esd :	0.00	0.00	0.00	0.00	0.00
Zero :	1.90000	3.85000	9.03000	0.00000	0.00000
Sigmas :	0.00000	0.00000	0.00000	0.00000	0.00000
Shift/esd :	0.00	0.00	0.00	0.00	0.00

Dif. Cons. Sum(shift/error)**2 :   0.00

Profile coefficients for histogram no. 1 and for phase no. 1:

Coeff. :	alp	be-0	be-1	sg-0	sg-1	sg-2	ga-0	ga-1	ga-2	gsf
Value :	2.898E-01	5.288E-02	7.468E-03	0.000E+00	2.460E+01	2.080E+00	0.000E+00	3.151E+00	0.000E+00	0.000E+00
Sigmas :					8.514E-01			1.560E-01		
Shift/esd:					0.00			0.00		

Coeff. :	g1ec	g2ec	rstr	rsta	rsca	L11	L22	L33	L12	L13
Value :	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Sigmas :										
Shift/esd:										

Coeff. :	L23
Value :	0.000E+00
Sigmas :	
Shift/esd:	

Profile coefficients for histogram no. 2 and for phase no. 1:

Coeff. :	alp	be-0	be-1	sg-0	sg-1	sg-2	ga-0	ga-1	ga-2	gsf
Value :	4.108E+00	6.789E-02	2.857E-03	3.543E+00	4.379E+01	-1.859E+00	0.000E+00	4.552E-02	1.628E+00	0.000E+00
Sigmas :					7.582E-01			1.182E-01		
Shift/esd:					0.00			0.00		

Coeff. :	g1ec	g2ec	rstr	rsta	rsca	L11	L22	L33	L12	L13
Value :	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Sigmas :										
Shift/esd:										

Coeff. :	L23
Value :	0.000E+00
Sigmas :	
Shift/esd:	

```
 Profile coefficients for histogram no.  3 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.469E-01
 Shift/esd:                                                  0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
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 Profile coefficients for histogram no.  1 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.514E-01                        1.560E-01
 Shift/esd:                                                  0.00                            0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.552E-02  1.628E+00
0.000E+00
 Sigmas   :                                              7.582E-01                        1.182E-01
 Shift/esd:                                                  0.00                            0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.469E-01
 Shift/esd:                                                  0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
 Profile coef. sum(shift/error)**2 :      0.00
```

```
 Background coefficients for histogram no.  1:
 Param.   :          1             2             3             4             5             6
 Coeff.   :   3.304123E-01  -1.782618E-02   5.276417E-02  -1.854789E-02  -9.835359E-03  -3.959241E-02
 Sigmas   :   4.614038E-03   8.661773E-03   7.904032E-03   7.311805E-03   6.852603E-03   6.160611E-03
 Shift/esd:          0.00          0.00          0.00          0.00          0.00          0.00
 Param.   :          7             8             9
 Coeff.   :  -1.854025E-02  -1.532352E-02  -7.139436E-03
 Sigmas   :   5.221992E-03   3.640604E-03   1.897094E-03
 Shift/esd:          0.00          0.00          0.00
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 Background coefficients for histogram no.  2:
 Param.   :          1             2             3             4             5             6
 Coeff.   :   2.736598E-01  -9.805781E-02   9.486720E-03  -1.770797E-02   1.124194E-02  -8.159674E-03
 Sigmas   :   2.500237E-03   4.625451E-03   4.215770E-03   3.985937E-03   3.837719E-03   3.726863E-03
 Shift/esd:          0.00          0.00          0.00          0.00          0.00          0.00
 Param.   :          7             8             9            10            11            12
 Coeff.   :   1.406928E-04  -1.500917E-02  -7.035227E-03   1.817594E-03   3.531192E-03  -1.696704E-02
 Sigmas   :   3.603154E-03   3.500098E-03   3.258470E-03   2.870660E-03   2.146295E-03   1.151934E-03
 Shift/esd:          0.00          0.00          0.00          0.00          0.01          0.01
 Background coef. sum(shift/error)**2 :      0.00

 CPU times for matrix build     1.56 sec; matrix inversion     0.00 sec
 Final variable sum((shift/esd)**2) for cycle1162:       0.10 Time:    1.56 sec
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 Restraint data statistics:
 No restraints used

 Powder data statistics                Fitted         -Bknd          pFree                  Average
              Bank Ndata Sum(w*d**2)  wRp     Rp    wRp     Rp    wRp     Rp  Npfree  DWd  Integral
 Hstgm  1 PNT   1  4524  4592.7     0.0694 0.1159 3.0075 0.6137 0.0000 0.0000     0   0.658   0.982
 Hstgm  2 PNT   2  3753  4940.9     0.0449 0.0945 0.1091 0.1135 0.0000 0.0000     0   0.462   0.990
 Hstgm  3 PNT   3  4808  4302.9     0.1278 0.1742 3.2083 0.7146 0.0000 0.0000     0   0.733   0.997
 Powder totals    13085  13836.     0.0614 0.1237 1.9003 0.4462 0.0000 0.0000     0   0.611

 No serial correlation in fit at 90% confidence for 1.952 < DWd < 2.048
 Cycle1163 There were  13085 observations.
 Total before-cycle CHI**2 (offset/sig) = 1.3836E+04 ( 4.9187E+00)
 Reduced CHI**2 =  1.061     for   43 variables

 Reflection data statistics
 Histogram  1  Type PNT   Nobs = 1302 R(F**2) =  0.1148
 Histogram  2  Type PNT   Nobs = 1071 R(F**2) =  0.0982
 Histogram  3  Type PNT   Nobs =  857 R(F**2) =  0.0805
 After matrix normalization and Marquardt modification:

    1 Columns of the    43 Column matrix are 0.0
 Full matrix recip. condition value & -log10 =   0.2036E-03      3.69
         Variable NoVarabl was not refined

 The value of the determinant is  1.2832*10.0**(   -22)

 Atom parameters for phase no. 1
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
 SC+3  (  1) Values  : 0.460  0.000000  0.000000  0.047678    0.359
             Sigmas  :                             0.000050    0.032
             Shft/esd:                               -0.03    -0.15
 Sc1      moved  0.00A     sum(shift/e.s.d)**2 :    0.02

 FE+3  (  2) Values  : 0.460  0.000000  0.000000  0.257903    0.535
             Sigmas  :                                       0.036
             Shft/esd:                                        0.16
 Fe1      moved  0.00A     sum(shift/e.s.d)**2 :    0.02

 O     (  3) Values  : 1.000  0.342324 -0.026074  0.817581    0.486
             Sigmas  :        0.000389  0.000227  0.000226    0.010
             Shft/esd:          -0.01      0.00      0.04     0.03
 O1       moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  4) Values  : 0.540  0.000000  0.000000  0.047678    0.359
```

```
            Sigmas  :                              0.000050    0.032
            Shft/esd:                                 -0.03    -0.15
 Fe2      moved  0.00A     sum(shift/e.s.d)**2 :    0.02

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 SC+3  (  5) Values  : 0.540  0.000000  0.000000  0.257903    0.535
            Sigmas  :                                       0.036
            Shft/esd:                                        0.16
 Sc2      moved  0.00A     sum(shift/e.s.d)**2 :    0.02

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 1 :      0.10
 Calculated unit cell formula weight:   892.800, density:  4.513gm/cm**3

 Atom parameters for phase no. 2
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
                                 Mx        My        Mz     |Moment|   Theta    Psi
 FE+3  (  1) Values  : 0.460  0.000000  0.000000  0.257890    0.535
            Sigmas  :                                       0.036
            Shft/esd:                                        0.16

 FE+3  (  1) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                         0.043    0.000    0.000
            Shft/esd:            0.00
 FE1      moved  0.00A     sum(shift/e.s.d)**2 :    0.02

 FE+3  (  2) Values  : 0.460  0.666670  0.333330  0.591220    0.535
            Sigmas  :                                       0.036
            Shft/esd:                                        0.16

 FE+3  (  2) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                         0.043    0.000    0.000
            Shft/esd:            0.00
 FE2      moved  0.00A     sum(shift/e.s.d)**2 :    0.02

 FE+3  (  3) Values  : 0.460  0.333330  0.666670  0.924560    0.535
            Sigmas  :                                       0.036
            Shft/esd:                                        0.16

 FE+3  (  3) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                         0.043    0.000    0.000
            Shft/esd:            0.00
 FE3      moved  0.00A     sum(shift/e.s.d)**2 :    0.02

 FE+3  (  4) Values  : 0.460  0.000000  0.000000  0.757890    0.535
            Sigmas  :                                       0.036
            Shft/esd:                                        0.16

 FE+3  (  4) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                         0.043    0.000    0.000
            Shft/esd:            0.00
 FE4      moved  0.00A     sum(shift/e.s.d)**2 :    0.02

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 FE+3  (  5) Values  : 0.460  0.666670  0.333330  0.091220    0.535
            Sigmas  :                                       0.036
            Shft/esd:                                        0.16

 FE+3  (  5) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                         0.043    0.000    0.000
            Shft/esd:            0.00
 FE5      moved  0.00A     sum(shift/e.s.d)**2 :    0.02

 FE+3  (  6) Values  : 0.460  0.333330  0.666670  0.424560    0.535
            Sigmas  :                                       0.036
            Shft/esd:                                        0.16

 FE+3  (  6) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                         0.043    0.000    0.000
            Shft/esd:            0.00
 FE6      moved  0.00A     sum(shift/e.s.d)**2 :    0.02
```

```
 FE+3  (  7) Values  : 0.540  0.000000  0.000000  0.047678    0.359
             Sigmas  :                             0.000050    0.032
             Shft/esd:                               -0.03    -0.15

 FE+3  (  7) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                         0.043    0.000    0.000
             Shft/esd:            0.00
 FE7      moved  0.00A     sum(shift/e.s.d)**2 :    0.02

 FE+3  (  8) Values  : 0.540  0.666670  0.333330  0.381008    0.359
             Sigmas  :                             0.000050    0.032
             Shft/esd:                               -0.03    -0.15

 FE+3  (  8) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                         0.043    0.000    0.000
             Shft/esd:            0.00
 FE8      moved  0.00A     sum(shift/e.s.d)**2 :    0.02

 FE+3  (  9) Values  : 0.540  0.333330  0.666670  0.714349    0.359
             Sigmas  :                             0.000050    0.032
             Shft/esd:                               -0.03    -0.15

 FE+3  (  9) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                         0.043    0.000    0.000
             Shft/esd:            0.00
 FE9      moved  0.00A     sum(shift/e.s.d)**2 :    0.02

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 FE+3  ( 10) Values  : 0.540  0.000000  0.000000  0.547679    0.359
             Sigmas  :                             0.000050    0.032
             Shft/esd:                               -0.03    -0.15

 FE+3  ( 10) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                         0.043    0.000    0.000
             Shft/esd:            0.00
 FE10     moved  0.00A     sum(shift/e.s.d)**2 :    0.02

 FE+3  ( 11) Values  : 0.540  0.666670  0.333330  0.881009    0.359
             Sigmas  :                             0.000050    0.032
             Shft/esd:                               -0.03    -0.15

 FE+3  ( 11) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                         0.043    0.000    0.000
             Shft/esd:            0.00
 FE11     moved  0.00A     sum(shift/e.s.d)**2 :    0.02

 FE+3  ( 12) Values  : 0.540  0.333330  0.666670  0.214349    0.359
             Sigmas  :                             0.000050    0.032
             Shft/esd:                               -0.03    -0.15

 FE+3  ( 12) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                         0.043    0.000    0.000
             Shft/esd:            0.00
 FE12     moved  0.00A     sum(shift/e.s.d)**2 :    0.02

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 2 :      0.29
 Calculated unit cell formula weight:   335.082, density:  1.694gm/cm**3

 Histogram scale factors:

 Histogram:    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 Scale    :    8.77263        8.78017        10.0722        0.00000        0.00000
 Sigmas   :   0.331840E-01   0.300370E-01   0.362686E-01    0.00000        0.00000
 Shift/esd:       0.02           0.02           0.01           0.00           0.00
 Histogram scale factor sum(shift/error)**2 :      0.00

 Lattice parameters for powder data:
 Phase  1
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202475  5.202475 14.014489    90.000    90.000   120.000     328.494
 Sigmas   :  0.000004  0.000004  0.000114     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
```

Phase 2

	a	b	c	alpha	beta	gamma	volume
Value :	5.202432	5.202446	14.014500	90.000	90.000	119.999	328.494
Sigmas :	0.000007	0.000007	0.000114	0.000	0.000	0.000	0.003

Recprocal metric tensor shift factor = 100%
Recprocal metric tensor sum(shift/error)**2 : 0.00

Diffractometer coefficients for powder data:

Histogram :	1 PNT	2 PNT	3 PNT	4 PNT*	5 PXC*
C/L1/R/2Th:	4569.20	6162.13	2139.59	0.00000	0.00000
Sigmas :	0.105501	0.00000	0.153602	0.00000	0.00000
Shift/esd :	0.00	0.00	0.00	0.00	0.00
Dif A/Pola:	-0.970206	-2.51000	1.29548	0.00000	0.00000
Sigmas :	0.627762E-01	0.00000	0.698622E-01	0.00000	0.00000
Shift/esd :	0.00	0.00	0.00	0.00	0.00
Zero :	1.90000	3.85000	9.03000	0.00000	0.00000
Sigmas :	0.00000	0.00000	0.00000	0.00000	0.00000
Shift/esd :	0.00	0.00	0.00	0.00	0.00

Dif. Cons. Sum(shift/error)**2 : 0.00

Profile coefficients for histogram no. 1 and for phase no. 1:

Coeff. :	alp	be-0	be-1	sg-0	sg-1	sg-2	ga-0	ga-1	ga-2	gsf
Value :	2.898E-01	5.288E-02	7.468E-03	0.000E+00	2.460E+01	2.080E+00	0.000E+00	3.151E+00	0.000E+00	0.000E+00
Sigmas :					8.514E-01			1.560E-01		
Shift/esd:					0.00			0.00		

Coeff. :	g1ec	g2ec	rstr	rsta	rsca	L11	L22	L33	L12	L13
Value :	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Sigmas :										
Shift/esd:										

Coeff. :	L23
Value :	0.000E+00
Sigmas :	
Shift/esd:	

Profile coefficients for histogram no. 2 and for phase no. 1:

Coeff. :	alp	be-0	be-1	sg-0	sg-1	sg-2	ga-0	ga-1	ga-2	gsf
Value :	4.108E+00	6.789E-02	2.857E-03	3.543E+00	4.379E+01	-1.859E+00	0.000E+00	4.546E-02	1.628E+00	0.000E+00
Sigmas :					7.582E-01			1.182E-01		
Shift/esd:					0.00			0.00		

Coeff. :	g1ec	g2ec	rstr	rsta	rsca	L11	L22	L33	L12	L13
Value :	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Sigmas :										
Shift/esd:										

Coeff. :	L23
Value :	0.000E+00
Sigmas :	
Shift/esd:	

Profile coefficients for histogram no. 3 and for phase no. 1:

Coeff. :	alp	be-0	be-1	sg-0	sg-1	sg-2	ga-0	ga-1	ga-2	gsf
Value :	1.000E+00	5.279E-02	2.026E-01	2.192E+01	7.865E+01	1.284E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Sigmas :					8.469E-01					
Shift/esd:					0.00					

Coeff. :	g1ec	g2ec	rstr	rsta	rsca	L11	L22	L33	L12	L13
Value :	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Sigmas :										
Shift/esd:										

Coeff. :	L23
Value :	0.000E+00
Sigmas :	
Shift/esd:	

Profile coefficients for histogram no. 1 and for phase no. 2:

Coeff.	alp	be-0	be-1	sg-0	sg-1	sg-2	ga-0	ga-1	ga-2	gsf
Value	2.898E-01	5.288E-02	7.468E-03	0.000E+00	2.460E+01	2.080E+00	0.000E+00	3.151E+00	0.000E+00	0.000E+00
Sigmas					8.514E-01			1.560E-01		
Shift/esd:					0.00			0.00		

Coeff.	g1ec	g2ec	rstr	rsta	rsca	L11	L22	L33	L12	L13
Value	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Sigmas										
Shift/esd:										

Coeff.	L23
Value	0.000E+00
Sigmas	
Shift/esd:	

Profile coefficients for histogram no. 2 and for phase no. 2:

Coeff.	alp	be-0	be-1	sg-0	sg-1	sg-2	ga-0	ga-1	ga-2	gsf
Value	4.108E+00	6.789E-02	2.857E-03	3.543E+00	4.379E+01	-1.859E+00	0.000E+00	4.546E-02	1.628E+00	0.000E+00
Sigmas					7.582E-01			1.182E-01		
Shift/esd:					0.00			0.00		

Coeff.	g1ec	g2ec	rstr	rsta	rsca	L11	L22	L33	L12	L13
Value	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Sigmas										
Shift/esd:										

Coeff.	L23
Value	0.000E+00
Sigmas	
Shift/esd:	

Profile coefficients for histogram no. 3 and for phase no. 2:

Coeff.	alp	be-0	be-1	sg-0	sg-1	sg-2	ga-0	ga-1	ga-2	gsf
Value	1.000E+00	5.279E-02	2.026E-01	2.192E+01	7.865E+01	1.284E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Sigmas					8.469E-01					
Shift/esd:					0.00					

Coeff.	g1ec	g2ec	rstr	rsta	rsca	L11	L22	L33	L12	L13
Value	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
Sigmas										
Shift/esd:										

Coeff.	L23
Value	0.000E+00
Sigmas	
Shift/esd:	

Profile coef. sum(shift/error)**2 : 0.00

Background coefficients for histogram no. 1:

Param.	1	2	3	4	5	6
Coeff.	3.304043E-01	-1.781903E-02	5.274485E-02	-1.854025E-02	-9.852714E-03	-3.959006E-02
Sigmas	4.614010E-03	8.661788E-03	7.903948E-03	7.311772E-03	6.852489E-03	6.160582E-03
Shift/esd:	0.00	0.00	0.00	0.00	0.00	0.00

Param.	7	8	9
Coeff.	-1.855682E-02	-1.532663E-02	-7.145601E-03
Sigmas	5.221907E-03	3.640604E-03	1.897053E-03
Shift/esd:	0.00	0.00	0.00

Background coefficients for histogram no. 2:

Param.	1	2	3	4	5	6
Coeff.	2.736550E-01	-9.805607E-02	9.474765E-03	-1.770668E-02	1.123327E-02	-8.159537E-03
Sigmas	2.500132E-03	4.625358E-03	4.215625E-03	3.985908E-03	3.837671E-03	3.726899E-03

```
 Shift/esd:           0.00           0.00           0.00           0.00           0.00           0.00
 Param.   :           7              8              9             10             11             12
 Coeff.   :   1.342611E-04  -1.501863E-02  -7.044830E-03   1.807270E-03   3.521173E-03  -1.697878E-02
 Sigmas   :   3.603158E-03   3.500127E-03   3.258467E-03   2.870652E-03   2.146261E-03   1.151844E-03
 Shift/esd:           0.00           0.00           0.00           0.00           0.00          -0.01
 Background coef. sum(shift/error)**2 :      0.00

 CPU times for matrix build     1.59 sec; matrix inversion     0.00 sec
 Final variable sum((shift/esd)**2) for cycle1163:       0.05 Time:    1.59 sec
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 Restraint data statistics:
 No restraints used

 Powder data statistics                Fitted         -Bknd          pFree                  Average
              Bank Ndata Sum(w*d**2)  wRp     Rp    wRp     Rp    wRp     Rp  Npfree  DWd  Integral
 Hstgm  1 PNT   1  4524  4592.5     0.0694 0.1159 3.0073 0.6137 0.0000 0.0000     0   0.658   0.982
 Hstgm  2 PNT   2  3753  4940.8     0.0449 0.0945 0.1091 0.1135 0.0000 0.0000     0   0.462   0.990
 Hstgm  3 PNT   3  4808  4303.0     0.1278 0.1742 3.2083 0.7146 0.0000 0.0000     0   0.732   0.997
 Powder totals    13085  13836.     0.0614 0.1237 1.9002 0.4462 0.0000 0.0000     0   0.611

 No serial correlation in fit at 90% confidence for 1.952 < DWd < 2.048
 Cycle1164 There were  13085 observations.
 Total before-cycle CHI**2 (offset/sig) = 1.3836E+04 ( 4.9186E+00)
 Reduced CHI**2 =  1.061     for   43 variables

 Reflection data statistics
 Histogram  1  Type PNT   Nobs = 1302 R(F**2) =  0.1148
 Histogram  2  Type PNT   Nobs = 1071 R(F**2) =  0.0982
 Histogram  3  Type PNT   Nobs =  857 R(F**2) =  0.0805
 After matrix normalization and Marquardt modification:

    1 Columns of the    43 Column matrix are 0.0
 Full matrix recip. condition value & -log10 =   0.2035E-03      3.69
         Variable NoVarabl was not refined

 The value of the determinant is  1.2970*10.0**(   -22)

 Atom parameters for phase no. 1
                      frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
 SC+3  (  1) Values  : 0.460  0.000000  0.000000  0.047680    0.363
             Sigmas  :                             0.000050    0.032
             Shft/esd:                                0.03     0.11
 Sc1       moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  2) Values  : 0.460  0.000000  0.000000  0.257903    0.531
             Sigmas  :                                        0.035
             Shft/esd:                                       -0.12
 Fe1       moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 O     (  3) Values  : 1.000  0.342325 -0.026073  0.817574    0.486
             Sigmas  :        0.000389  0.000228  0.000227    0.010
             Shft/esd:           0.00      0.00     -0.03    -0.02
 O1        moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  4) Values  : 0.540  0.000000  0.000000  0.047680    0.363
             Sigmas  :                             0.000050    0.032
             Shft/esd:                                0.03     0.11
 Fe2       moved  0.00A     sum(shift/e.s.d)**2 :    0.01

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 SC+3  (  5) Values  : 0.540  0.000000  0.000000  0.257903    0.531
             Sigmas  :                                        0.035
             Shft/esd:                                       -0.12
 Sc2       moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 1 :      0.06
 Calculated unit cell formula weight:   892.800, density:  4.513gm/cm**3

 Atom parameters for phase no. 2
```

```
                    frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
                                Mx        My        Mz     |Moment|   Theta    Psi
 FE+3  (  1) Values  : 0.460  0.000000  0.000000  0.257890    0.531
             Sigmas  :                                      0.035
             Shft/esd:                                      -0.12

 FE+3  (  1) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE1       moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  2) Values  : 0.460  0.666670  0.333330  0.591220    0.531
             Sigmas  :                                      0.035
             Shft/esd:                                      -0.12

 FE+3  (  2) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE2       moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  3) Values  : 0.460  0.333330  0.666670  0.924560    0.531
             Sigmas  :                                      0.035
             Shft/esd:                                      -0.12

 FE+3  (  3) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE3       moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  4) Values  : 0.460  0.000000  0.000000  0.757890    0.531
             Sigmas  :                                      0.035
             Shft/esd:                                      -0.12

 FE+3  (  4) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE4       moved  0.00A     sum(shift/e.s.d)**2 :    0.01

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 FE+3  (  5) Values  : 0.460  0.666670  0.333330  0.091220    0.531
             Sigmas  :                                      0.035
             Shft/esd:                                      -0.12

 FE+3  (  5) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE5       moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  6) Values  : 0.460  0.333330  0.666670  0.424560    0.531
             Sigmas  :                                      0.035
             Shft/esd:                                      -0.12

 FE+3  (  6) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE6       moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  7) Values  : 0.540  0.000000  0.000000  0.047680    0.363
             Sigmas  :                              0.000050    0.032
             Shft/esd:                                  0.03     0.11

 FE+3  (  7) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE7       moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  8) Values  : 0.540  0.666670  0.333330  0.381010    0.363
             Sigmas  :                              0.000050    0.032
             Shft/esd:                                  0.03     0.11

 FE+3  (  8) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
```

```
 FE8      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  9) Values  : 0.540  0.333330  0.666670  0.714351    0.363
             Sigmas  :                            0.000050    0.032
             Shft/esd:                               0.03     0.11

 FE+3  (  9) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE9      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

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 FE+3  ( 10) Values  : 0.540  0.000000  0.000000  0.547681    0.363
             Sigmas  :                            0.000050    0.032
             Shft/esd:                               0.03     0.11

 FE+3  ( 10) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE10     moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  ( 11) Values  : 0.540  0.666670  0.333330  0.881011    0.363
             Sigmas  :                            0.000050    0.032
             Shft/esd:                               0.03     0.11

 FE+3  ( 11) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE11     moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  ( 12) Values  : 0.540  0.333330  0.666670  0.214351    0.363
             Sigmas  :                            0.000050    0.032
             Shft/esd:                               0.03     0.11

 FE+3  ( 12) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE12     moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 2 :      0.16
 Calculated unit cell formula weight:   335.082, density:  1.694gm/cm**3

 Histogram scale factors:

 Histogram:    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 Scale    :    8.77223        8.77968        10.0718        0.00000        0.00000
 Sigmas   :   0.332055E-01   0.300699E-01   0.362803E-01    0.00000        0.00000
 Shift/esd:      -0.01          -0.02          -0.01           0.00           0.00
 Histogram scale factor sum(shift/error)**2 :      0.00

 Lattice parameters for powder data:
 Phase  1
               a         b         c       alpha     beta      gamma     volume
 Value    :  5.202475  5.202475 14.014489    90.000    90.000   120.000     328.494
 Sigmas   :  0.000004  0.000004  0.000114     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Phase  2
               a         b         c       alpha     beta      gamma     volume
 Value    :  5.202432  5.202446 14.014500    90.000    90.000   119.999     328.494
 Sigmas   :  0.000007  0.000007  0.000114     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Recprocal metric tensor sum(shift/error)**2 :      0.00
1SF0                                                          GENLES   Version Win32  Jun 24 14:07:39 2011
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 Diffractometer coefficients for powder data:
 Histogram :    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 C/L1/R/2Th:    4569.20        6162.13        2139.59        0.00000        0.00000
 Sigmas    :   0.105500        0.00000       0.153604        0.00000        0.00000
 Shift/esd :       0.00           0.00           0.00           0.00           0.00
 Dif A/Pola:  -0.970092       -2.51000        1.29553        0.00000        0.00000
 Sigmas    :   0.627747E-01    0.00000       0.698621E-01    0.00000        0.00000
```

```
 Shift/esd :       0.00          0.00          0.00          0.00          0.00
 Zero      :    1.90000       3.85000       9.03000       0.00000       0.00000
 Sigmas    :    0.00000       0.00000       0.00000       0.00000       0.00000
 Shift/esd :       0.00          0.00          0.00          0.00          0.00
 Dif. Cons. Sum(shift/error)**2 :      0.00

 Profile coefficients for histogram no.  1 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.514E-01                        1.560E-01
 Shift/esd:                                                  0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.550E-02  1.628E+00
0.000E+00
 Sigmas   :                                              7.582E-01                        1.182E-01
 Shift/esd:                                                  0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.469E-01
 Shift/esd:                                                  0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
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 Profile coefficients for histogram no.  1 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.514E-01                        1.560E-01
 Shift/esd:                                                  0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
```

```
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.550E-02  1.628E+00
0.000E+00
 Sigmas   :                                             7.582E-01                        1.182E-01
 Shift/esd:                                                 0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                             8.469E-01
 Shift/esd:                                                 0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
 Profile coef. sum(shift/error)**2 :      0.00

 Background coefficients for histogram no.  1:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   3.304095E-01  -1.782464E-02   5.275792E-02  -1.854620E-02  -9.840911E-03  -3.959202E-02
 Sigmas   :   4.613965E-03   8.661647E-03   7.903880E-03   7.311704E-03   6.852506E-03   6.160570E-03
 Shift/esd:           0.00          0.00          0.00          0.00          0.00          0.00
 Param.   :           7             8             9
 Coeff.   :  -1.854514E-02  -1.532443E-02  -7.141201E-03
 Sigmas   :   5.221954E-03   3.640598E-03   1.897082E-03
 Shift/esd:           0.00          0.00          0.00
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 Background coefficients for histogram no.  2:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   2.736583E-01  -9.805709E-02   9.483268E-03  -1.770733E-02   1.123947E-02  -8.159399E-03
 Sigmas   :   2.500233E-03   4.625442E-03   4.215748E-03   3.985926E-03   3.837702E-03   3.726864E-03
 Shift/esd:           0.00          0.00          0.00          0.00          0.00          0.00
 Param.   :           7             8             9            10            11            12
 Coeff.   :   1.389942E-04  -1.501151E-02  -7.037697E-03   1.814924E-03   3.528515E-03  -1.697022E-02
 Sigmas   :   3.603153E-03   3.500113E-03   3.258482E-03   2.870671E-03   2.146293E-03   1.151913E-03
 Shift/esd:           0.00          0.00          0.00          0.00          0.00          0.01
 Background coef. sum(shift/error)**2 :      0.00

 CPU times for matrix build     1.59 sec; matrix inversion     0.02 sec
 Final variable sum((shift/esd)**2) for cycle1164:       0.03 Time:    1.61 sec
1SFO                                                          GENLES   Version Win32  Jun 24 14:07:39 2011
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 Restraint data statistics:
 No restraints used

 Powder data statistics                Fitted         -Bknd          pFree                  Average
```

```
             Bank Ndata Sum(w*d**2)  wRp     Rp    wRp     Rp    wRp     Rp  Npfree  DWd  Integral
 Hstgm  1 PNT   1  4524  4592.6     0.0694 0.1159 3.0074 0.6137 0.0000 0.0000     0   0.658   0.982
 Hstgm  2 PNT   2  3753  4940.9     0.0449 0.0945 0.1091 0.1135 0.0000 0.0000     0   0.462   0.990
 Hstgm  3 PNT   3  4808  4302.9     0.1278 0.1742 3.2083 0.7146 0.0000 0.0000     0   0.732   0.997
 Powder totals    13085  13836.     0.0614 0.1237 1.9003 0.4462 0.0000 0.0000     0   0.611

 No serial correlation in fit at 90% confidence for 1.952 < DWd < 2.048
 Cycle1165 There were  13085 observations.
 Total before-cycle CHI**2 (offset/sig) = 1.3836E+04 ( 4.9185E+00)
 Reduced CHI**2 =  1.061     for   43 variables

 Reflection data statistics
 Histogram  1  Type PNT   Nobs = 1302 R(F**2) =  0.1148
 Histogram  2  Type PNT   Nobs = 1071 R(F**2) =  0.0982
 Histogram  3  Type PNT   Nobs =  857 R(F**2) =  0.0805
 After matrix normalization and Marquardt modification:

    1 Columns of the    43 Column matrix are 0.0
 Full matrix recip. condition value & -log10 =   0.2036E-03      3.69
        Variable NoVarabl was not refined

 The value of the determinant is  1.2863*10.0**(   -22)

 Atom parameters for phase no. 1
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
 SC+3  (  1) Values  : 0.460  0.000000  0.000000  0.047679    0.360
             Sigmas  :                             0.000050    0.032
             Shft/esd:                               -0.02    -0.08
 Sc1      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  2) Values  : 0.460  0.000000  0.000000  0.257903    0.534
             Sigmas  :                                       0.036
             Shft/esd:                                        0.08
 Fe1      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 O     (  3) Values  : 1.000  0.342324 -0.026074  0.817579    0.486
             Sigmas  :        0.000389  0.000227  0.000226    0.010
             Shft/esd:           0.00      0.00      0.02     0.01
 O1       moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  4) Values  : 0.540  0.000000  0.000000  0.047679    0.360
             Sigmas  :                             0.000050    0.032
             Shft/esd:                               -0.02    -0.08
 Fe2      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

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 SC+3  (  5) Values  : 0.540  0.000000  0.000000  0.257903    0.534
             Sigmas  :                                       0.036
             Shft/esd:                                        0.08
 Sc2      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 1 :      0.03
 Calculated unit cell formula weight:   892.800, density:  4.513gm/cm**3

 Atom parameters for phase no. 2
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
                                 Mx        My        Mz     |Moment|   Theta    Psi
 FE+3  (  1) Values  : 0.460  0.000000  0.000000  0.257890    0.534
             Sigmas  :                                       0.036
             Shft/esd:                                        0.08

 FE+3  (  1) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE1      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  2) Values  : 0.460  0.666670  0.333330  0.591220    0.534
             Sigmas  :                                       0.036
             Shft/esd:                                        0.08

 FE+3  (  2) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
```

```
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE2      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  3) Values  : 0.460  0.333330  0.666670  0.924560    0.534
            Sigmas  :                                       0.036
            Shft/esd:                                        0.08

 FE+3  (  3) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE3      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  4) Values  : 0.460  0.000000  0.000000  0.757890    0.534
            Sigmas  :                                       0.036
            Shft/esd:                                        0.08

 FE+3  (  4) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE4      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

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 FE+3  (  5) Values  : 0.460  0.666670  0.333330  0.091220    0.534
            Sigmas  :                                       0.036
            Shft/esd:                                        0.08

 FE+3  (  5) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE5      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  6) Values  : 0.460  0.333330  0.666670  0.424560    0.534
            Sigmas  :                                       0.036
            Shft/esd:                                        0.08

 FE+3  (  6) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE6      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  7) Values  : 0.540  0.000000  0.000000  0.047679    0.360
            Sigmas  :                               0.000050    0.032
            Shft/esd:                                  -0.02    -0.08

 FE+3  (  7) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE7      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  8) Values  : 0.540  0.666670  0.333330  0.381009    0.360
            Sigmas  :                               0.000050    0.032
            Shft/esd:                                  -0.02    -0.08

 FE+3  (  8) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE8      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  (  9) Values  : 0.540  0.333330  0.666670  0.714350    0.360
            Sigmas  :                               0.000050    0.032
            Shft/esd:                                  -0.02    -0.08

 FE+3  (  9) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
            Sigmas  :           0.043                        0.043    0.000    0.000
            Shft/esd:            0.00
 FE9      moved  0.00A     sum(shift/e.s.d)**2 :    0.01

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 FE+3  ( 10) Values  : 0.540  0.000000  0.000000  0.547680    0.360
            Sigmas  :                               0.000050    0.032
            Shft/esd:                                  -0.02    -0.08
```

```
 FE+3  ( 10) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE10     moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  ( 11) Values  : 0.540  0.666670  0.333330  0.881010    0.360
             Sigmas  :                             0.000050    0.032
             Shft/esd:                               -0.02    -0.08

 FE+3  ( 11) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE11     moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 FE+3  ( 12) Values  : 0.540  0.333330  0.666670  0.214350    0.360
             Sigmas  :                             0.000050    0.032
             Shft/esd:                               -0.02    -0.08

 FE+3  ( 12) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE12     moved  0.00A     sum(shift/e.s.d)**2 :    0.01

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 2 :      0.09
 Calculated unit cell formula weight:   335.082, density:  1.694gm/cm**3

 Histogram scale factors:

 Histogram:    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 Scale    :    8.77253        8.78005        10.0721        0.00000        0.00000
 Sigmas   :   0.331897E-01   0.300458E-01   0.362717E-01    0.00000        0.00000
 Shift/esd:       0.01           0.01           0.01           0.00           0.00
 Histogram scale factor sum(shift/error)**2 :      0.00

 Lattice parameters for powder data:
 Phase  1
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202475  5.202475 14.014489    90.000    90.000   120.000     328.494
 Sigmas   :  0.000004  0.000004  0.000114     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Phase  2
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202432  5.202446 14.014500    90.000    90.000   119.999     328.494
 Sigmas   :  0.000007  0.000007  0.000114     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Recprocal metric tensor sum(shift/error)**2 :      0.00
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 Diffractometer coefficients for powder data:
 Histogram :    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 C/L1/R/2Th:    4569.20        6162.13        2139.59        0.00000        0.00000
 Sigmas    :   0.105500        0.00000       0.153602        0.00000        0.00000
 Shift/esd :       0.00           0.00           0.00           0.00           0.00
 Dif A/Pola:  -0.970171       -2.51000        1.29552        0.00000        0.00000
 Sigmas    :   0.627756E-01    0.00000       0.698619E-01    0.00000        0.00000
 Shift/esd :       0.00           0.00           0.00           0.00           0.00
 Zero      :    1.90000        3.85000        9.03000        0.00000        0.00000
 Sigmas    :    0.00000        0.00000        0.00000        0.00000        0.00000
 Shift/esd :       0.00           0.00           0.00           0.00           0.00
 Dif. Cons. Sum(shift/error)**2 :      0.00

 Profile coefficients for histogram no.  1 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.514E-01                        1.560E-01
 Shift/esd:                                                  0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
```

```
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.548E-02  1.628E+00
0.000E+00
 Sigmas   :                                              7.582E-01                         1.182E-01
 Shift/esd:                                                  0.00                              0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.469E-01
 Shift/esd:                                                  0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
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 Profile coefficients for histogram no.  1 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.514E-01                         1.560E-01
 Shift/esd:                                                  0.00                              0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.548E-02  1.628E+00
0.000E+00
 Sigmas   :                                              7.582E-01                         1.182E-01
 Shift/esd:                                                  0.00                              0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
```

```
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                             8.469E-01
 Shift/esd:                                                  0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
 Profile coef. sum(shift/error)**2 :      0.00

 Background coefficients for histogram no.  1:
 Param.   :           1              2              3              4              5              6
 Coeff.   :   3.304054E-01  -1.782049E-02   5.274797E-02  -1.854159E-02  -9.849624E-03  -3.959022E-02
 Sigmas   :   4.613941E-03   8.661622E-03   7.903878E-03   7.311721E-03   6.852528E-03   6.160629E-03
 Shift/esd:           0.00           0.00           0.00           0.00           0.00           0.00
 Param.   :           7              8              9
 Coeff.   :  -1.855364E-02  -1.532588E-02  -7.144468E-03
 Sigmas   :   5.221975E-03   3.640631E-03   1.897068E-03
 Shift/esd:           0.00           0.00           0.00
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 Background coefficients for histogram no.  2:
 Param.   :           1              2              3              4              5              6
 Coeff.   :   2.736558E-01  -9.805617E-02   9.476895E-03  -1.770665E-02   1.123486E-02  -8.159340E-03
 Sigmas   :   2.500217E-03   4.625475E-03   4.215742E-03   3.985945E-03   3.837685E-03   3.726868E-03
 Shift/esd:           0.00           0.00           0.00           0.00           0.00           0.00
 Param.   :           7              8              9             10             11             12
 Coeff.   :   1.355629E-04  -1.501663E-02  -7.042864E-03   1.809344E-03   3.523126E-03  -1.697653E-02
 Sigmas   :   3.603138E-03   3.500117E-03   3.258470E-03   2.870659E-03   2.146270E-03   1.151864E-03
 Shift/esd:           0.00           0.00           0.00           0.00           0.00          -0.01
 Background coef. sum(shift/error)**2 :      0.00

 CPU times for matrix build     1.72 sec; matrix inversion     0.02 sec
 Final variable sum((shift/esd)**2) for cycle1165:       0.02 Time:    1.73 sec
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 Restraint data statistics:
 No restraints used

 Powder data statistics                Fitted         -Bknd          pFree                  Average
              Bank Ndata Sum(w*d**2)  wRp     Rp    wRp     Rp    wRp     Rp  Npfree  DWd  Integral
 Hstgm  1 PNT   1  4524  4592.6     0.0694 0.1159 3.0073 0.6137 0.0000 0.0000     0   0.658   0.982
 Hstgm  2 PNT   2  3753  4940.8     0.0449 0.0945 0.1091 0.1135 0.0000 0.0000     0   0.462   0.990
 Hstgm  3 PNT   3  4808  4303.0     0.1278 0.1742 3.2083 0.7146 0.0000 0.0000     0   0.732   0.997
 Powder totals    13085  13836.     0.0614 0.1237 1.9002 0.4462 0.0000 0.0000     0   0.611

 No serial correlation in fit at 90% confidence for 1.952 < DWd < 2.048
 Cycle1166 There were  13085 observations.
 Total before-cycle CHI**2 (offset/sig) = 1.3836E+04 ( 4.9187E+00)
 Reduced CHI**2 =  1.061     for   43 variables

 Reflection data statistics
 Histogram  1  Type PNT   Nobs = 1302 R(F**2) =  0.1148
 Histogram  2  Type PNT   Nobs = 1071 R(F**2) =  0.0982
 Histogram  3  Type PNT   Nobs =  857 R(F**2) =  0.0805
 After matrix normalization and Marquardt modification:
```

```
   1 Columns of the    43 Column matrix are 0.0
 Full matrix recip. condition value & -log10 =   0.2035E-03      3.69
        Variable NoVarabl was not refined

 The value of the determinant is  1.2938*10.0**(   -22)

 Atom parameters for phase no. 1
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
 SC+3  (  1) Values  : 0.460  0.000000  0.000000  0.047679    0.362
             Sigmas  :                             0.000050    0.032
             Shft/esd:                                0.01     0.06
 Sc1      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  2) Values  : 0.460  0.000000  0.000000  0.257903    0.531
             Sigmas  :                                        0.036
             Shft/esd:                                       -0.06
 Fe1      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 O     (  3) Values  : 1.000  0.342325 -0.026073  0.817575    0.486
             Sigmas  :        0.000389  0.000228  0.000227    0.010
             Shft/esd:           0.00      0.00     -0.02    -0.01
 O1       moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  4) Values  : 0.540  0.000000  0.000000  0.047679    0.362
             Sigmas  :                             0.000050    0.032
             Shft/esd:                                0.01     0.06
 Fe2      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

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 SC+3  (  5) Values  : 0.540  0.000000  0.000000  0.257903    0.531
             Sigmas  :                                        0.036
             Shft/esd:                                       -0.06
 Sc2      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 1 :      0.02
 Calculated unit cell formula weight:   892.800, density:  4.513gm/cm**3

 Atom parameters for phase no. 2
                     frac       x         y         z     100*Uiso  100*U11  100*U22  100*U33  100*U12  100*U13
100*U23
                                Mx        My        Mz     |Moment|   Theta    Psi
 FE+3  (  1) Values  : 0.460  0.000000  0.000000  0.257890    0.531
             Sigmas  :                                        0.036
             Shft/esd:                                       -0.06

 FE+3  (  1) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE1      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  2) Values  : 0.460  0.666670  0.333330  0.591220    0.531
             Sigmas  :                                        0.036
             Shft/esd:                                       -0.06

 FE+3  (  2) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE2      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  3) Values  : 0.460  0.333330  0.666670  0.924560    0.531
             Sigmas  :                                        0.036
             Shft/esd:                                       -0.06

 FE+3  (  3) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
             Sigmas  :           0.043                        0.043    0.000    0.000
             Shft/esd:            0.00
 FE3      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  4) Values  : 0.460  0.000000  0.000000  0.757890    0.531
             Sigmas  :                                        0.036
             Shft/esd:                                       -0.06
```

```
 FE+3  (  4) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.00
 FE4       moved  0.00A     sum(shift/e.s.d)**2 :    0.00

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 FE+3  (  5) Values  : 0.460  0.666670  0.333330  0.091220    0.531
              Sigmas  :                                     0.036
              Shft/esd:                                     -0.06

 FE+3  (  5) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.00
 FE5       moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  6) Values  : 0.460  0.333330  0.666670  0.424560    0.531
              Sigmas  :                                     0.036
              Shft/esd:                                     -0.06

 FE+3  (  6) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.00
 FE6       moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  7) Values  : 0.540  0.000000  0.000000  0.047679    0.362
              Sigmas  :                             0.000050    0.032
              Shft/esd:                                0.01     0.06

 FE+3  (  7) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.00
 FE7       moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  8) Values  : 0.540  0.666670  0.333330  0.381009    0.362
              Sigmas  :                             0.000050    0.032
              Shft/esd:                                0.01     0.06

 FE+3  (  8) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.00
 FE8       moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  (  9) Values  : 0.540  0.333330  0.666670  0.714350    0.362
              Sigmas  :                             0.000050    0.032
              Shft/esd:                                0.01     0.06

 FE+3  (  9) Moments :          -2.670     0.000     0.000    2.670   90.000  180.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.00
 FE9       moved  0.00A     sum(shift/e.s.d)**2 :    0.00

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 FE+3  ( 10) Values  : 0.540  0.000000  0.000000  0.547680    0.362
              Sigmas  :                             0.000050    0.032
              Shft/esd:                                0.01     0.06

 FE+3  ( 10) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.00
 FE10      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  ( 11) Values  : 0.540  0.666670  0.333330  0.881010    0.362
              Sigmas  :                             0.000050    0.032
              Shft/esd:                                0.01     0.06

 FE+3  ( 11) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
              Sigmas  :           0.043                       0.043    0.000    0.000
              Shft/esd:            0.00
 FE11      moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 FE+3  ( 12) Values  : 0.540  0.333330  0.666670  0.214350    0.362
              Sigmas  :                             0.000050    0.032
```

```
            Shft/esd:                                0.01     0.06

 FE+3  ( 12) Moments :           2.670     0.000     0.000    2.670   90.000    0.000
            Sigmas  :           0.043                         0.043    0.000    0.000
            Shft/esd:            0.00
 FE12     moved  0.00A     sum(shift/e.s.d)**2 :    0.00

 Maximum atom shift:   0.00
 Atomic parameter sum(shift/error)**2 for phase 2 :      0.05
 Calculated unit cell formula weight:   335.082, density:  1.694gm/cm**3

 Histogram scale factors:

 Histogram:    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 Scale    :    8.77231        8.77978        10.0719        0.00000        0.00000
 Sigmas   :   0.332014E-01   0.300636E-01   0.362781E-01    0.00000        0.00000
 Shift/esd:      -0.01          -0.01           0.00           0.00           0.00
 Histogram scale factor sum(shift/error)**2 :      0.00

 Lattice parameters for powder data:
 Phase  1
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202475  5.202475 14.014489    90.000    90.000   120.000     328.494
 Sigmas   :  0.000004  0.000004  0.000114     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Phase  2
                a         b         c       alpha     beta      gamma     volume
 Value    :  5.202432  5.202446 14.014500    90.000    90.000   119.999     328.494
 Sigmas   :  0.000007  0.000007  0.000114     0.000     0.000     0.000       0.003
 Recprocal metric tensor shift factor = 100%
 Recprocal metric tensor sum(shift/error)**2 :      0.00
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 Diffractometer coefficients for powder data:
 Histogram :    1  PNT         2  PNT         3  PNT         4  PNT*        5  PXC*
 C/L1/R/2Th:    4569.20        6162.13        2139.59        0.00000        0.00000
 Sigmas    :   0.105500        0.00000       0.153604        0.00000        0.00000
 Shift/esd :       0.00           0.00           0.00           0.00           0.00
 Dif A/Pola:  -0.970103       -2.51000        1.29551        0.00000        0.00000
 Sigmas    :   0.627750E-01    0.00000       0.698621E-01    0.00000        0.00000
 Shift/esd :       0.00           0.00           0.00           0.00           0.00
 Zero      :    1.90000        3.85000        9.03000        0.00000        0.00000
 Sigmas    :    0.00000        0.00000        0.00000        0.00000        0.00000
 Shift/esd :       0.00           0.00           0.00           0.00           0.00
 Dif. Cons. Sum(shift/error)**2 :      0.00

 Profile coefficients for histogram no.  1 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
0.000E+00
 Sigmas   :                                              8.514E-01                        1.560E-01
 Shift/esd:                                                  0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.550E-02  1.628E+00
0.000E+00
 Sigmas   :                                              7.582E-01                        1.182E-01
 Shift/esd:                                                  0.00                             0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
```

```
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  1:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                             8.469E-01
 Shift/esd:                                                 0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
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 Profile coefficients for histogram no.  1 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  2.898E-01  5.288E-02  7.468E-03  0.000E+00  2.460E+01  2.080E+00  0.000E+00  3.151E+00  0.000E+00
0.000E+00
 Sigmas   :                                             8.514E-01                        1.560E-01
 Shift/esd:                                                 0.00                            0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  2 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  4.108E+00  6.789E-02  2.857E-03  3.543E+00  4.379E+01 -1.859E+00  0.000E+00  4.550E-02  1.628E+00
0.000E+00
 Sigmas   :                                             7.582E-01                        1.182E-01
 Shift/esd:                                                 0.00                            0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:

 Profile coefficients for histogram no.  3 and for phase no.  2:
 Coeff.   :    alp        be-0       be-1       sg-0       sg-1       sg-2       ga-0       ga-1       ga-2
gsf
 Value    :  1.000E+00  5.279E-02  2.026E-01  2.192E+01  7.865E+01  1.284E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
 Sigmas   :                                             8.469E-01
 Shift/esd:                                                 0.00
 Coeff.   :    g1ec       g2ec       rstr       rsta       rsca       L11        L22        L33        L12
L13
 Value    :  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
0.000E+00
```

```
 Sigmas   :
 Shift/esd:
 Coeff.   :    L23
 Value    :  0.000E+00
 Sigmas   :
 Shift/esd:
 Profile coef. sum(shift/error)**2 :      0.00

 Background coefficients for histogram no.  1:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   3.304084E-01  -1.782352E-02   5.275507E-02  -1.854489E-02  -9.843285E-03  -3.959142E-02
 Sigmas   :   4.613899E-03   8.661540E-03   7.903750E-03   7.311590E-03   6.852414E-03   6.160526E-03
 Shift/esd:           0.00          0.00          0.00          0.00          0.00          0.00
 Param.   :           7             8             9
 Coeff.   :  -1.854736E-02  -1.532476E-02  -7.142101E-03
 Sigmas   :   5.221928E-03   3.640597E-03   1.897076E-03
 Shift/esd:           0.00          0.00          0.00
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 Background coefficients for histogram no.  2:
 Param.   :           1             2             3             4             5             6
 Coeff.   :   2.736576E-01  -9.805672E-02   9.481514E-03  -1.770705E-02   1.123820E-02  -8.159352E-03
 Sigmas   :   2.500226E-03   4.625457E-03   4.215746E-03   3.985926E-03   3.837695E-03   3.726873E-03
 Shift/esd:           0.00          0.00          0.00          0.00          0.00          0.00
 Param.   :           7             8             9            10            11            12
 Coeff.   :   1.380600E-04  -1.501287E-02  -7.039095E-03   1.813455E-03   3.527101E-03  -1.697187E-02
 Sigmas   :   3.603161E-03   3.500121E-03   3.258479E-03   2.870661E-03   2.146283E-03   1.151899E-03
 Shift/esd:           0.00          0.00          0.00          0.00          0.00          0.00
 Background coef. sum(shift/error)**2 :      0.00

 CPU times for matrix build     1.67 sec; matrix inversion     0.02 sec
 Final variable sum((shift/esd)**2) for cycle1166:       0.01 Time:    1.69 sec

 Convergence was achieved
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                  |----------------------------------------|
                  |     Program PUBTABLES Version Win32    |
                  |  Generate crystal structure data tables |
                  | Distributed on Wed Jun 01 16:54:19 2011 |
                  |----------------------------------------|

        |---------------------------------------------------------------|
        |            Allen C. Larson and Robert B. Von Dreele           |
        |      Manuel Lujan, Jr. Neutron Scattering Center, MS-H805     |
        |      Los Alamos National Laboratory, Los Alamos, NM  87545    |
        |                                                               |
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        |---------------------------------------------------------------|

 The last history record is :
     HSTRY 90 GENLES  Win32  Jun 24 14:07:40 2011 Sdsq= 0.138E+05 S/E= 0.863E-02

------------------------------------------------
     Archiving SAFE_NEUTRON_FINAL_STEPHANSS.EXP as SAFE_NEUTRON_FINAL_STEPHANSS.007
------------------------------------------------


------------------------------------------------
     Archiving SAFE_NEUTRON_FINAL_STEPHANSS.EXP as SAFE_NEUTRON_FINAL_STEPHANSS.008
------------------------------------------------
```