```
flipsub 4F7O.mtz DANO=DANO_x1 weak=0.2 name=CSN5 trial=10

 ================================================
 !   Substructure determination by Charge flipping  !
 !           version  february  19,  2013           !
 ================================================

 Checking input parameters


----------------  Crystal data ------------------
mtzin file            .......   4F7O.mtz
label for Delta-Ano   .......   DANO_x1
local normalization   .......   yes
generic name          .......   CSN5
dmin resolution limit .......   2.60 A
dmax resolution limit .......   20.0 A
unit cell parameters  .......   161.7336 46.5050 71.2613 90.0000 100.2653
90.0000
SG symmetry number    .......   5

----------------  CF parameters used  ----------
ked coefficient        .......   1.2
weak threshold         .......   0.2
convergence mode       .......   symmetry
convergence threshold .......   85.0
maximum cycles / trial ......   2000
additional cycles      .......   50
polishing LDE cycles   ........  50
number of repeated trials ....  10  sumgood
-------------------------------------------------

Press ENTER to continue


************************************************************
                      Superflip
                  Version: 09/05/11 14:22
Palatinus, L. & Chapuis, G.(2007): J. Appl. Cryst. 40, 786-790
             http://superspace.epfl.ch/superflip
************************************************************


---------------------------------------------
Start of the calculation: 19.FEB 2013, 12:36:03
---------------------------------------------

######################################################################
# Following data were read from the input file or set as default: #
######################################################################

Job title: Substructure determination by Charge Flipping web1

------------------------
Information about files:
------------------------
Name of the input file: CSN5.inflip
Density will be writen in ccp4 format to file   CSN5.map
Warning: If the outputfile exists, it will be overwritten by the new density.
```

Commentaire:
input command line

Commentaire:
input MTZ file, SAD dataset
DANO_x1 column = anomalous differences

Commentaire:
data included up to 2.6 A resolution

Commentaire:
charge flipping parameters
ked=1.2
weak=0.2

Commentaire:
Symmetry score threshold used to detect convergence

Commentaire:
10 independent trials
densities from the successful trials are summed up and an average density is written out at the end of the procedure (CSN5.map)

```
Logfile will contain only basic information about the calculation.
Logfile will contain information about the data coverage.

-----------------------------
Crystallographic information:
-----------------------------
Superspace dimension:             3
Dimension of the physical space:  3
Direct cell parameters:         161.734   46.505   71.261   90.000  100.265
90.00  Volume:     527406.8
Reciprocal cell parameters:       0.006    0.022    0.014   90.000   79.735
90.00  Volume:          0.0
2 symmetry operations found, their list follows:

   1:   1  0  0   0.0000   2:  -1  0  0   0.0000
        0  1  0   0.0000        0  1  0   0.0000
        0  0  1   0.0000        0  0 -1   0.0000

The structure is non-centrosymmetric.
The symmetry operations are to be combined with the following centering vectors:
   0.0000   0.0000   0.0000
   0.5000   0.5000   0.0000


--------------------------
Settings of the algorithm:
--------------------------
Number of voxels:                  120    36    60   Total:    259200
Number of voxels for polishing:    180    54    81   Total:    787320
The density modification method will be charge flipping.
Delta:    1.200
  Static delta will be used: pixels with density below   1.200*sigma(map) will
be flipped in each cycle.
The iteration will be stopped when the convergence is detected or after  2000
cycles.
After the detection of convergence   50 cycles of iteration will be added.
After the regular iteration  50 cycles of "density polishing" will be applied.
The random number generator will be initialized automatically.
The whole calculation will be repeated 10times.
 10 densities with the best R-value will be saved with the names bestXX_YYYY,
where XX is the serial number and YYYY is the name of the output density given
by user.

Random initial phases will be assigned to the structure factors.
Isotropic Debye-Waller factor:   0.000
Proportion of reflections to be treated as weak:   0.200
Only reflections with d >     2.60 and d <    20.00 will be used.
All reflections with d >     3.38 not present in the input data set will be
treated a missing.
The normalized amplitudes of the missing reflections will be constrained to less
than  4.0.

The resulting density will be shifted and averaged according to the symmetry
operations given above.
Following symmetry operations will be used to locate the origin of symmetry:   2

#################################
# Information about reflections: #
#################################
```

Commentaire:
input ked parameter

Commentaire:
maximum number of cycles per trial

Commentaire:
input weak parameter

Number of reflections in the input file: 13903
Maximum indices in expanded reflection set: 58 16 26

Number of reflections treated as missing: 1245

F**2 statistics:

SHELL	NO OF REFLS	RESOLUTION	MEAN DSTAR^3	MEAN F^2	SMOOTHED F^2
1	384	10.21	0.000535	5734.	4503.
2	386	8.30	0.001346	3496.	3987.
3	378	7.31	0.002157	2894.	2730.
4	386	6.67	0.002968	1746.	2162.
5	420	6.21	0.003778	1985.	1814.
6	388	5.85	0.004589	1655.	1887.
7	410	5.56	0.005400	2097.	1908.
8	414	5.33	0.006211	1910.	1798.
9	422	5.13	0.007022	1351.	1560.
10	418	4.95	0.007833	1489.	1407.
11	416	4.80	0.008644	1353.	1288.
....					
12	392	4.66	0.009455	1000.	1167.
54	410	2.83	0.043514	450.	515.
55	436	2.82	0.044325	567.	533.
56	414	2.80	0.045135	570.	547.
57	416	2.78	0.045946	497.	514.
58	386	2.77	0.046757	482.	479.
59	364	2.75	0.047568	458.	480.
60	338	2.74	0.048379	508.	476.
61	316	2.72	0.049190	453.	459.
62	368	2.71	0.050001	419.	448.
63	346	2.69	0.050812	481.	480.
64	278	2.68	0.051623	542.	491.
65	274	2.66	0.052434	435.	457.
66	342	2.65	0.053245	402.	426.
67	294	2.64	0.054056	449.	457.
68	260	2.63	0.054867	522.	473.
69	280	2.61	0.055677	432.	489.
70	260	2.60	0.056488	532.	477.

E**2 statistics from Karle normalization:

SHELL	NO OF REFLS	RESOLUTION	MEAN DSTAR^3	MEAN E^2
1	384	10.21	0.000535	1.281
2	386	8.30	0.001346	0.894
3	378	7.31	0.002157	1.037
4	386	6.67	0.002968	0.799
5	420	6.21	0.003778	1.081
6	388	5.85	0.004589	0.879
7	410	5.56	0.005400	1.104
8	414	5.33	0.006211	1.066
9	422	5.13	0.007022	0.864
10	418	4.95	0.007833	1.062
11	416	4.80	0.008644	1.056
12	392	4.66	0.009455	0.851
13	434	4.54	0.010266	1.037
.....				
61	316	2.72	0.049190	0.988
62	368	2.71	0.050001	0.928
63	346	2.69	0.050812	1.009
64	278	2.68	0.051623	1.109
65	274	2.66	0.052434	0.952
66	342	2.65	0.053245	0.931
67	294	2.64	0.054056	0.992
68	260	2.63	0.054867	1.102
69	280	2.61	0.055677	0.886
70	260	2.60	0.056488	1.118

<E**2>_pseudo = 1.000

Commentaire: end of normalization step: locally normalized |E| values

```
-----------------------------------------------------------
Coverage statistics of the expanded reflections by shells:
-----------------------------------------------------------
Resolution (sin(th)/l):    0.050    0.100    0.150    0.192
Resolution (d_min):       10.000    5.000    3.333    2.600
Obs. refl. in shell:         412     3510     9922    14256
Total refl. in shell:        574     3936    10613    16644
Coverage in shell:         71.8%    89.2%    93.5%    85.7%
Commulative coverage:      71.8%    87.0%    91.5%    88.5%


#############
# Iteration #
#############

Estimated delta:  0.0004
Random seed:     123604848

Current k_ed =    1.20000  (absolute delta =   0.00054)
   10  R: 70.240  Charge:      79.96   Peaks:  1.00  Sym:100.00   Score:    ---
   20  R: 69.760  Charge:      78.73   Peaks:  1.16  Sym:100.00   Score:    ---
   30  R: 70.580  Charge:      77.41   Peaks:  1.27  Sym:100.00   Score:    ---
   40  R: 70.327  Charge:      76.51   Peaks:  1.30  Sym:100.00   Score:    ---
   50  R: 70.130  Charge:      76.57   Peaks:  1.47  Sym: 98.12   Score:    ---
   60  R: 70.397  Charge:      75.93   Peaks:  1.45  Sym: 98.12   Score:    ---
   70  R: 70.046  Charge:      76.00   Peaks:  1.49  Sym: 98.12   Score:    ---
   80  R: 70.055  Charge:      75.56   Peaks:  1.53  Sym: 98.12   Score:    ---
   90  R: 70.090  Charge:      76.12   Peaks:  1.48  Sym: 98.12   Score:    ---
  100  R: 70.312  Charge:      75.52   Peaks:  1.56  Sym: 97.76   Score:    ---
  200  R: 70.466  Charge:      75.26   Peaks:  1.73  Sym: 96.54   Score:    ---
  300  R: 70.760  Charge:      74.90   Peaks:  1.72  Sym: 96.23   Score:    ---
  400  R: 71.235  Charge:      74.18   Peaks:  2.01  Sym: 90.19   Score:    ---
  500  R: 70.387  Charge:      71.52   Peaks:  2.54  Sym: 81.14   Score:    ---

Calculation successfully converged after   550 cycles.
Last iteration record:
  550  R: 71.020  Charge:      71.15   Peaks:  2.74  Sym: 81.14   Score:    ---

    50 cycles of noise suppression follow:
   10  R: 53.772  Charge:       0.00   Peaks:  9.36
   20  R: 53.871  Charge:       0.00   Peaks: 10.94
   30  R: 53.939  Charge:       0.00   Peaks: 11.55
   40  R: 54.055  Charge:       0.00   Peaks: 11.85
   50  R: 54.209  Charge:       0.00   Peaks: 12.04

####################################
# Checking the density for symmetry #
####################################

Centering vectors:
  0.000  0.000  0.000
  0.500  0.500  0.000

Symmetry operations compatible with the lattice and centering:
                          Symmetry operation             agreement factor
       2(0,1,0):          -x1          x2          -x3    9.583    XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
       m(0,1,0):           x1          -x2          x3   77.903    XXXXXXX
            -1:           -x1          -x2          -x3  80.268    XXXXX
       c(0,1,0):           x1          -x2        1/2+x3 96.783    XX
```

Commentaire:
convergence detected Sym<85

Commentaire: control on the quality of the map obtained by CF: the symmetry is derived from theP1 map (independent of the input SG symmetry information).

```
------------------------------------------------
Space group derived from the symmetry operations:
------------------------------------------------
    HM symbol:      C2
    Hall symbol:    c 2y
    Fingerprint:    33121060qW0 (0,0,0)
    Centering vectors:
      0.000  0.000  0.000
      0.500  0.500  0.000
    Symmetry operations:
              1:            x1           x2           x3
       2(0,1,0):           -x1           x2          -x3


##########################################
# Search for the origin of the space group #
##########################################


Position of the origin in the CF map:
  0.7487  0.0000  0.5975
Agreement factors of individual generators:
Number smb agreement
   2   2        9.59

Overall agreement factor:    9.59

You can obtain more information about the reconstructed reflection phases by
using 'expandedlog yes'.

Properties of the saved densities:
  Nr. Run   Rvalue    Peaks   Symm.     Der.SG
    1   1   54.21    12.04    9.59         C2

Current density added to the averaged density. Number of averaged densities:   1

Run number  1. Still  9 to go.


#############
# Iteration #
#############

Estimated delta:  0.0004
Random seed:     123620232

Current k_ed =    1.20000  (absolute delta =   0.00054)
   10  R: 70.309  Charge:      81.41   Peaks:  1.00  Sym:100.00   Score:    ---
   20  R: 69.730  Charge:      78.58   Peaks:  1.24  Sym:100.00   Score:    ---
   30  R: 70.074  Charge:      77.71   Peaks:  1.29  Sym:100.00   Score:    ---
   40  R: 69.931  Charge:      77.04   Peaks:  1.38  Sym:100.00   Score:    ---
   50  R: 70.080  Charge:      76.82   Peaks:  1.43  Sym: 98.36   Score:    ---
   60  R: 70.342  Charge:      76.78   Peaks:  1.48  Sym: 98.36   Score:    ---
   70  R: 70.438  Charge:      76.07   Peaks:  1.49  Sym: 98.36   Score:    ---
   80  R: 69.894  Charge:      77.22   Peaks:  1.52  Sym: 98.36   Score:    ---
   90  R: 69.937  Charge:      76.29   Peaks:  1.56  Sym: 98.36   Score:    ---
  100  R: 70.393  Charge:      75.63   Peaks:  1.60  Sym: 96.95   Score:    ---
  200  R: 70.524  Charge:      74.36   Peaks:  1.76  Sym: 95.67   Score:    ---
  300  R: 70.400  Charge:      73.46   Peaks:  1.99  Sym: 98.78   Score:    ---
```

Commentaire: The derived space group is the same as the input SG=5

Commentaire:
The P1 map is now constrained to obey the **input XL symmetry** properties: the agreement score is good <10-15

Commentaire:
final score for the first successful trial. The substructure density map file best01_CSN5.map is written out.

Commentaire:
Next trial with a new random seed

```
  400   R: 70.856  Charge:      73.77   Peaks:  1.92  Sym: 96.30   Score:    ---
  500   R: 71.136  Charge:      73.70   Peaks:  2.01  Sym: 95.09   Score:    ---
  600   R: 71.146  Charge:      73.01   Peaks:  2.10  Sym: 96.37   Score:    ---
  700   R: 71.129  Charge:      73.30   Peaks:  1.93  Sym: 95.58   Score:    ---
  800   R: 70.742  Charge:      73.06   Peaks:  2.08  Sym: 96.97   Score:    ---
  900   R: 71.043  Charge:      72.57   Peaks:  2.02  Sym: 96.22   Score:    ---
 1000   R: 71.372  Charge:      73.15   Peaks:  2.24  Sym: 97.10   Score:    ---
 2000   R: 70.803  Charge:      72.37   Peaks:  2.14  Sym: 96.21   Score:    ---

Calculation is finished. No convergence was detected after  2000 cycles.
Last iteration record:
 2000   R: 70.803  Charge:      72.37   Peaks:  2.14  Sym: 96.21   Score:    ---

    50 cycles of noise suppression follow:
   10   R: 54.652  Charge:       0.00   Peaks:  4.42
   20   R: 54.803  Charge:       0.00   Peaks:  5.03
   30   R: 54.850  Charge:       0.00   Peaks:  5.35
   40   R: 54.785  Charge:       0.00   Peaks:  5.56
   50   R: 54.785  Charge:       0.00   Peaks:  5.70
The density was aligned with the reference file, agreement   75.09%.
Shift:   0.35383  0.48942  0.37967


####################################
# Checking the density for symmetry #
####################################

Centering vectors:
  0.000  0.000  0.000
  0.500  0.500  0.000

Symmetry operations compatible with the lattice and centering:
                        Symmetry operation            agreement factor
      m(0,1,0):           x1         -x2          x3   16.532    xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
           -1:          -x1         -x2         -x3   87.940    xxxxx
      2(0,1,0):         -x1          x2         -x3   89.073    xxxxx
      c(0,1,0):          x1         -x2       1/2+x3   99.155    x

-------------------------------------------------
Space group derived from the symmetry operations:
-------------------------------------------------
    HM symbol:      Cm
    Hall symbol:    C -2y
    Fingerprint:    33121063}20 (0,0,0)
    Centering vectors:
      0.000  0.000  0.000
      0.500  0.500  0.000
    Symmetry operations:
               1:            x1           x2           x3
        m(0,1,0):            x1          -x2           x3


#########################################
# Search for the origin of the space group #
#########################################


Position of the origin in the CF map:
  0.0000  0.0000  0.0060
Agreement factors of individual generators:
Number smb agreement
```

Commentaire:
No convergence detected
Sym-score >85.

Commentaire:
impossible to detect C2
symmetry operators in the P1 map

```
   2   2       89.00

Overall agreement factor:  89.07

You can obtain more information about the reconstructed reflection phases by
using 'expandedlog yes'.

Properties of the saved densities:
  Nr. Run   Rvalue    Peaks   Symm.     Der.SG
   1   1    54.21    12.04    9.59         C2
   2   2    54.79     5.70   89.07         Cm

Run number  2. Still  8 to go.


#############
# Iteration #
#############

Estimated delta:  0.0004
Random seed:     123704304

Current k_ed =    1.20000  (absolute delta =   0.00054)
   10  R: 70.265  Charge:      80.12   Peaks:  1.00  Sym:100.00   Score:    ---
   20  R: 70.441  Charge:      78.48   Peaks:  1.13  Sym:100.00   Score:    ---
   30  R: 69.935  Charge:      77.09   Peaks:  1.29  Sym:100.00   Score:    ---
   40  R: 70.594  Charge:      76.46   Peaks:  1.34  Sym:100.00   Score:    ---
   50  R: 70.378  Charge:      76.97   Peaks:  1.39  Sym: 96.53   Score:    ---
   60  R: 70.296  Charge:      76.77   Peaks:  1.38  Sym: 96.53   Score:    ---
   70  R: 70.750  Charge:      75.76   Peaks:  1.44  Sym: 96.53   Score:    ---
   80  R: 70.861  Charge:      75.25   Peaks:  1.48  Sym: 96.53   Score:    ---
   90  R: 70.910  Charge:      74.61   Peaks:  1.47  Sym: 96.53   Score:    ---
  100  R: 70.334  Charge:      75.16   Peaks:  1.51  Sym: 97.80   Score:    ---
  200  R: 70.465  Charge:      74.48   Peaks:  1.69  Sym: 96.13   Score:    ---
  300  R: 70.684  Charge:      73.52   Peaks:  1.71  Sym: 96.14   Score:    ---
  400  R: 70.685  Charge:      73.30   Peaks:  1.72  Sym: 96.45   Score:    ---
  500  R: 70.614  Charge:      73.43   Peaks:  1.88  Sym: 95.36   Score:    ---
  600  R: 70.803  Charge:      73.13   Peaks:  1.83  Sym: 96.99   Score:    ---
  700  R: 71.083  Charge:      71.60   Peaks:  2.02  Sym: 96.29   Score:    ---
  800  R: 71.217  Charge:      72.26   Peaks:  2.06  Sym: 95.21   Score:    ---
  900  R: 70.503  Charge:      71.89   Peaks:  2.00  Sym: 98.29   Score:    ---
 1000  R: 71.368  Charge:      71.63   Peaks:  2.04  Sym: 97.29   Score:    ---
 2000  R: 71.567  Charge:      71.98   Peaks:  2.00  Sym: 96.92   Score:    ---

Calculation is finished. No convergence was detected after  2000 cycles.
Last iteration record:
 2000  R: 71.567  Charge:      71.98   Peaks:  2.00  Sym: 96.92   Score:    ---

    50 cycles of noise suppression follow:
   10  R: 55.240  Charge:       0.00   Peaks:  4.28
   20  R: 55.353  Charge:       0.00   Peaks:  4.77
   30  R: 55.397  Charge:       0.00   Peaks:  5.00
   40  R: 55.465  Charge:       0.00   Peaks:  5.17
   50  R: 55.450  Charge:       0.00   Peaks:  5.32
The density was aligned with the reference file, agreement   82.05%.
Shift:   0.84707  0.75817  0.47921


####################################
# Checking the density for symmetry #
```

Commentaire:
poor symmetry agreement factor

Commentaire:
Trial 2 unsuccessful.
The density map best02_CSN5.map is written out (but useless)

Commentaire:
Next trial with a new random seed

Commentaire:
No convergence detected
Sym-score >85.

```
####################################

Centering vectors:
  0.000  0.000  0.000
  0.500  0.500  0.000

Symmetry operations compatible with the lattice and centering:
                              Symmetry operation              agreement factor
      m(0,1,0):           x1         -x2          x3   16.692    xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
      2(0,1,0):          -x1          x2         -x3   89.882    xxxx
           -1:           -x1         -x2         -x3   89.962    xxxx
      c(0,1,0):           x1         -x2      1/2+x3   97.390    x

-------------------------------------------------
Space group derived from the symmetry operations:
-------------------------------------------------
    HM symbol:     Cm
    Hall symbol:   c -2y
    Fingerprint:   33121063}20 (0,0,0)
    Centering vectors:
      0.000  0.000  0.000
      0.500  0.500  0.000
    Symmetry operations:
               1:            x1           x2           x3
        m(0,1,0):            x1          -x2           x3


##########################################
# Search for the origin of the space group #
##########################################


Position of the origin in the CF map:
  0.0116  0.0000  0.0062
Agreement factors of individual generators:
Number smb agreement
   2   2       89.88

Overall agreement factor:  89.88

You can obtain more information about the reconstructed reflection phases by
using 'expandedlog yes'.

Properties of the saved densities:
  Nr. Run  Rvalue   Peaks  Symm.    Der.SG
   1   1   54.21   12.04   9.59        C2
   2   2   54.79    5.70  89.07        Cm
   3   3   55.45    5.32  89.88        Cm

Run number  3. Still  7 to go.


#############
# Iteration #
#############

Estimated delta:  0.0004
Random seed:     123747848

Current k_ed =    1.20000  (absolute delta =   0.00054)
   10  R: 70.167  Charge:      80.73   Peaks:  1.00  Sym:100.00   Score:    ---
```

Commentaire:
poor symmetry agreement factor

```
   20  R: 69.805  Charge:      79.26   Peaks:  1.12  Sym:100.00   Score:    ---
   30  R: 70.168  Charge:      78.41   Peaks:  1.30  Sym:100.00   Score:    ---
   40  R: 69.990  Charge:      76.67   Peaks:  1.38  Sym:100.00   Score:    ---
   50  R: 70.142  Charge:      77.19   Peaks:  1.40  Sym: 97.25   Score:    ---
   60  R: 70.394  Charge:      75.93   Peaks:  1.46  Sym: 97.25   Score:    ---
   70  R: 69.972  Charge:      75.25   Peaks:  1.51  Sym: 97.25   Score:    ---
   80  R: 70.371  Charge:      76.71   Peaks:  1.51  Sym: 97.25   Score:    ---
   90  R: 70.567  Charge:      76.60   Peaks:  1.47  Sym: 97.25   Score:    ---
  100  R: 70.251  Charge:      75.62   Peaks:  1.58  Sym: 99.51   Score:    ---
  200  R: 70.936  Charge:      74.41   Peaks:  1.81  Sym: 95.75   Score:    ---
  300  R: 70.753  Charge:      74.51   Peaks:  1.81  Sym: 95.38   Score:    ---
  400  R: 71.382  Charge:      73.54   Peaks:  2.06  Sym: 95.49   Score:    ---
  500  R: 70.788  Charge:      72.64   Peaks:  2.08  Sym: 95.99   Score:    ---
  600  R: 71.086  Charge:      72.16   Peaks:  2.36  Sym: 95.04   Score:    ---
  700  R: 71.254  Charge:      72.50   Peaks:  2.16  Sym: 95.20   Score:    ---
  800  R: 70.440  Charge:      72.46   Peaks:  2.19  Sym: 94.18   Score:    ---
  900  R: 70.580  Charge:      72.32   Peaks:  2.11  Sym: 92.76   Score:    ---
 1000  R: 70.271  Charge:      72.07   Peaks:  2.16  Sym: 92.35   Score:    ---
 2000  R: 71.210  Charge:      72.16   Peaks:  2.30  Sym: 91.92   Score:    ---

Calculation is finished. No convergence was detected after  2000 cycles.
Last iteration record:
 2000  R: 71.210  Charge:      72.16   Peaks:  2.30  Sym: 91.92   Score:    ---

    50 cycles of noise suppression follow:
   10  R: 54.816  Charge:       0.00   Peaks:  5.45
   20  R: 54.713  Charge:       0.00   Peaks:  6.35
   30  R: 54.767  Charge:       0.00   Peaks:  6.87
   40  R: 54.900  Charge:       0.00   Peaks:  7.22
   50  R: 55.047  Charge:       0.00   Peaks:  7.50
The density was aligned with the reference file, agreement   55.72%.
Shift:   0.23643  0.29962  0.42917


####################################
# Checking the density for symmetry #
####################################

Centering vectors:
  0.000  0.000  0.000
  0.500  0.500  0.000

Symmetry operations compatible with the lattice and centering:
                          Symmetry operation            agreement factor
      m(0,1,0):           x1         -x2          x3   12.778    xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
      2(0,1,0):          -x1          x2         -x3   76.714    xxxxxxxxxx
           -1:           -x1         -x2         -x3   78.436    xxxxxxxxx
      c(0,1,0):           x1         -x2       1/2+x3   99.492    x

-------------------------------------------------
Space group derived from the symmetry operations:
-------------------------------------------------
    HM symbol:      Cm
    Hall symbol:    c -2y
    Fingerprint:    33121063}20 (0,0,0)
    Centering vectors:
      0.000  0.000  0.000
      0.500  0.500  0.000
    Symmetry operations:
              1:            x1           x2           x3
        m(0,1,0):           x1          -x2           x3
```

Commentaire: wrong symmetry

```
##########################################
# Search for the origin of the space group #
##########################################


Position of the origin in the CF map:
  0.0000  0.0000  0.0012
Agreement factors of individual generators:
Number smb agreement
   2   2       76.71

Overall agreement factor:  76.72

You can obtain more information about the reconstructed reflection phases by
using 'expandedlog yes'.

Properties of the saved densities:
  Nr. Run  Rvalue   Peaks  Symm.    Der.SG
   1   1   54.21   12.04   9.59        C2
   2   2   54.79    5.70  89.07        Cm
   3   3   55.45    5.32  89.88        Cm
   4   4   55.05    7.50  76.72        Cm

Run number  4. Still  6 to go.


#############
# Iteration #
#############

Estimated delta:  0.0004
Random seed:     123833112

Current k_ed =    1.20000  (absolute delta =   0.00054)
   10  R: 70.205  Charge:      80.22   Peaks:  1.00  Sym:100.00   Score:    ---
   20  R: 70.199  Charge:      79.03   Peaks:  1.14  Sym:100.00   Score:    ---
   30  R: 69.966  Charge:      78.13   Peaks:  1.15  Sym:100.00   Score:    ---
   40  R: 70.183  Charge:      77.70   Peaks:  1.25  Sym:100.00   Score:    ---
   50  R: 70.691  Charge:      76.73   Peaks:  1.30  Sym: 97.40   Score:    ---
   60  R: 70.240  Charge:      76.86   Peaks:  1.37  Sym: 97.40   Score:    ---
   70  R: 69.906  Charge:      76.59   Peaks:  1.36  Sym: 97.40   Score:    ---
   80  R: 69.775  Charge:      76.09   Peaks:  1.47  Sym: 97.40   Score:    ---
   90  R: 69.649  Charge:      75.97   Peaks:  1.51  Sym: 97.40   Score:    ---
  100  R: 70.415  Charge:      75.94   Peaks:  1.49  Sym: 96.19   Score:    ---
  200  R: 70.814  Charge:      73.38   Peaks:  1.95  Sym: 97.90   Score:    ---
  300  R: 70.814  Charge:      71.74   Peaks:  2.23  Sym: 94.45   Score:    ---
  400  R: 70.842  Charge:      72.20   Peaks:  2.23  Sym: 96.84   Score:    ---
  500  R: 70.794  Charge:      72.48   Peaks:  2.27  Sym: 93.96   Score:    ---
  600  R: 70.449  Charge:      71.98   Peaks:  2.41  Sym: 91.57   Score:    ---
  700  R: 70.953  Charge:      71.31   Peaks:  2.28  Sym: 93.57   Score:    ---
  800  R: 71.431  Charge:      72.66   Peaks:  2.34  Sym: 92.71   Score:    ---
  900  R: 70.977  Charge:      72.19   Peaks:  2.25  Sym: 93.55   Score:    ---
 1000  R: 71.058  Charge:      70.55   Peaks:  2.27  Sym: 92.82   Score:    ---
 2000  R: 70.985  Charge:      71.31   Peaks:  2.43  Sym: 95.48   Score:    ---

Calculation is finished. No convergence was detected after  2000 cycles.
Last iteration record:
 2000  R: 70.985  Charge:      71.31   Peaks:  2.43  Sym: 95.48   Score:    ---
```

Commentaire: poor symmetry agreement factor

```
    50 cycles of noise suppression follow:
   10  R: 55.116  Charge:       0.00   Peaks:  6.18
   20  R: 55.434  Charge:       0.00   Peaks:  7.56
   30  R: 55.851  Charge:       0.00   Peaks:  8.58
   40  R: 56.217  Charge:       0.00   Peaks:  9.62
   50  R: 56.524  Charge:       0.00   Peaks: 10.61
The density was aligned with the reference file, agreement   61.01%.
Shift:   0.45152  0.63070  0.02440


####################################

# Checking the density for symmetry #
####################################

Centering vectors:
  0.000  0.000  0.000
  0.500  0.500  0.000

Symmetry operations compatible with the lattice and centering:
                              Symmetry operation             agreement factor
      m(0,1,0):          x1         -x2          x3    9.960    xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
           -1:         -x1         -x2         -x3   81.166    xxxxxxx
      2(0,1,0):        -x1          x2         -x3   82.232    xxxxxxx
      c(0,1,0):          x1         -x2      1/2+x3   98.331    x

------------------------------------------------
Space group derived from the symmetry operations:
------------------------------------------------
    HM symbol:     Cm
    Hall symbol:   c -2y
    Fingerprint:   33121063}20 (0,0,0)
    Centering vectors:
      0.000  0.000  0.000
      0.500  0.500  0.000
    Symmetry operations:
               1:            x1           x2           x3
       m(0,1,0):            x1          -x2           x3


############################################
# Search for the origin of the space group #
############################################


Position of the origin in the CF map:
  0.9892  0.0000  0.1719
Agreement factors of individual generators:
Number smb agreement
   2   2       82.23

Overall agreement factor:  82.23

You can obtain more information about the reconstructed reflection phases by
using 'expandedlog yes'.

Properties of the saved densities:
  Nr. Run  Rvalue   Peaks  Symm.    Der.SG
   1   1   54.21   12.04    9.59       C2
   2   2   54.79    5.70   89.07       Cm
```

```
   3    3    55.45     5.32    89.88         Cm
   4    4    55.05     7.50    76.72         Cm
   5    5    56.52    10.61    82.23         Cm

Run number  5. Still  5 to go.


#############
# Iteration #
#############

Estimated delta:  0.0004
Random seed:     123918048

Current k_ed =    1.20000  (absolute delta =   0.00054)
   10  R: 70.012  Charge:      80.94   Peaks:  1.00  Sym:100.00   Score:    ---
   20  R: 70.010  Charge:      78.67   Peaks:  1.10  Sym:100.00   Score:    ---
   30  R: 69.966  Charge:      77.14   Peaks:  1.20  Sym:100.00   Score:    ---
   40  R: 70.299  Charge:      76.49   Peaks:  1.31  Sym:100.00   Score:    ---
   50  R: 70.238  Charge:      75.58   Peaks:  1.35  Sym: 96.02   Score:    ---
   60  R: 70.363  Charge:      75.94   Peaks:  1.36  Sym: 96.02   Score:    ---
   70  R: 70.523  Charge:      75.91   Peaks:  1.45  Sym: 96.02   Score:    ---
   80  R: 70.255  Charge:      75.23   Peaks:  1.51  Sym: 96.02   Score:    ---
   90  R: 70.413  Charge:      74.73   Peaks:  1.51  Sym: 96.02   Score:    ---
  100  R: 70.500  Charge:      74.67   Peaks:  1.58  Sym: 95.01   Score:    ---
  200  R: 70.863  Charge:      74.05   Peaks:  1.80  Sym: 94.56   Score:    ---
  300  R: 70.962  Charge:      73.87   Peaks:  1.83  Sym: 91.95   Score:    ---
  400  R: 71.352  Charge:      72.23   Peaks:  2.12  Sym: 86.51   Score:    ---
  500  R: 70.992  Charge:      71.06   Peaks:  2.57  Sym: 80.14   Score:    ---

Calculation successfully converged after   500 cycles.
Last iteration record:
  500  R: 70.992  Charge:      71.06   Peaks:  2.57  Sym: 80.14   Score:    ---

    50 cycles of noise suppression follow:
   10  R: 54.101  Charge:       0.00   Peaks:  8.25
   20  R: 53.999  Charge:       0.00   Peaks:  9.35
   30  R: 53.956  Charge:       0.00   Peaks:  9.81
   40  R: 54.010  Charge:       0.00   Peaks: 10.12
   50  R: 54.106  Charge:       0.00   Peaks: 10.36
The density was aligned with the reference file, agreement     8.60%.
Shift:   0.83524  0.74494  0.72779


####################################
# Checking the density for symmetry #
####################################

Centering vectors:
  0.000  0.000  0.000
  0.500  0.500  0.000

Symmetry operations compatible with the lattice and centering:
                              Symmetry operation              agreement factor
      2(0,1,0):          -x1          x2          -x3    9.858    xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
           -1:          -x1          -x2          -x3   79.153    xxxxxxxx
      m(0,1,0):           x1          -x2           x3   81.423    xxxxxxx
      c(0,1,0):           x1          -x2      1/2+x3   98.141    x

------------------------------------------------
Space group derived from the symmetry operations:
```

Commentaire:
good agreement with the first substructure map obtained in trial 1

```
-------------------------------------------------
    HM symbol:      C2
    Hall symbol:    c 2y
    Fingerprint:    33121060qW0 (0,0,0)
    Centering vectors:
      0.000  0.000  0.000
      0.500  0.500  0.000
    Symmetry operations:
              1:            x1           x2           x3
       2(0,1,0):           -x1           x2          -x3


##########################################
# Search for the origin of the space group #
##########################################


Position of the origin in the CF map:
  0.0000  0.0000  0.0000
Agreement factors of individual generators:
Number smb agreement
   2   2        9.86

Overall agreement factor:   9.86

You can obtain more information about the reconstructed reflection phases by
using 'expandedlog yes'.

Properties of the saved densities:
  Nr. Run  Rvalue   Peaks  Symm.    Der.SG
   1   1   54.21   12.04   9.59        C2
   2   2   54.79    5.70  89.07        Cm
   3   3   55.45    5.32  89.88        Cm
   4   4   55.05    7.50  76.72        Cm
   5   5   56.52   10.61  82.23        Cm
   6   6   54.11   10.36   9.86        C2

Current density added to the averaged density. Number of averaged densities:   2

Run number  6. Still  4 to go.


#############
# Iteration #
#############

Estimated delta:  0.0004
Random seed:     123933536

Current k_ed =    1.20000  (absolute delta =   0.00054)
   10  R: 69.925  Charge:      80.49   Peaks:  1.00  Sym:100.00   Score:    ---
   20  R: 70.371  Charge:      78.70   Peaks:  1.16  Sym:100.00   Score:    ---
   30  R: 70.186  Charge:      77.62   Peaks:  1.24  Sym:100.00   Score:    ---
   40  R: 70.237  Charge:      76.61   Peaks:  1.32  Sym:100.00   Score:    ---
   50  R: 69.939  Charge:      77.16   Peaks:  1.40  Sym: 99.24   Score:    ---
   60  R: 70.324  Charge:      76.88   Peaks:  1.44  Sym: 99.24   Score:    ---
   70  R: 70.377  Charge:      75.94   Peaks:  1.40  Sym: 99.24   Score:    ---
   80  R: 70.164  Charge:      76.87   Peaks:  1.40  Sym: 99.24   Score:    ---
   90  R: 70.271  Charge:      76.58   Peaks:  1.47  Sym: 99.24   Score:    ---
  100  R: 69.860  Charge:      75.39   Peaks:  1.52  Sym: 97.83   Score:    ---
```

Commentaire: The derived space group is the same as the input SG=5

Commentaire: summary for successful trial #6

```
  200   R: 70.585   Charge:      74.68    Peaks:  1.61   Sym: 97.30    Score:     ---
  300   R: 70.528   Charge:      74.57    Peaks:  1.69   Sym: 95.84    Score:     ---
  400   R: 70.942   Charge:      72.79    Peaks:  2.05   Sym: 94.76    Score:     ---
  500   R: 70.124   Charge:      73.93    Peaks:  2.01   Sym: 92.67    Score:     ---
  600   R: 70.353   Charge:      71.24    Peaks:  2.57   Sym: 79.61    Score:     ---

Calculation successfully converged after   650 cycles.
Last iteration record:
  650   R: 70.644   Charge:      70.87    Peaks:  2.76   Sym: 79.61    Score:     ---

    50 cycles of noise suppression follow:
   10   R: 53.848   Charge:       0.00    Peaks:  8.81
   20   R: 53.976   Charge:       0.00    Peaks: 10.26
   30   R: 54.082   Charge:       0.00    Peaks: 10.87
   40   R: 54.172   Charge:       0.00    Peaks: 11.21
   50   R: 54.226   Charge:       0.00    Peaks: 11.37
The density was aligned with the reference file, agreement    7.01%.
Shift:   0.10748  0.37428  0.10059


####################################
# Checking the density for symmetry #
####################################

Centering vectors:
  0.000  0.000  0.000
  0.500  0.500  0.000

Symmetry operations compatible with the lattice and centering:
                      Symmetry operation            agreement factor
      2(0,1,0):          -x1          x2         -x3   11.592    xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
      m(0,1,0):           x1         -x2          x3   79.250    xxxxxxx
           -1:           -x1         -x2         -x3   81.560    xxxxxx
      c(0,1,0):           x1         -x2       1/2+x3   98.781    x

------------------------------------------------
Space group derived from the symmetry operations:
------------------------------------------------
    HM symbol:     C2
    Hall symbol:   c 2y
    Fingerprint:   33121060qW0 (0,0,0)
    Centering vectors:
      0.000  0.000  0.000
      0.500  0.500  0.000
    Symmetry operations:
               1:            x1           x2           x3
       2(0,1,0):           -x1           x2          -x3


#########################################
# Search for the origin of the space group #
#########################################


Position of the origin in the CF map:
  0.0000  0.0000  0.0000
Agreement factors of individual generators:
Number smb agreement
   2   2       11.59

Overall agreement factor:  11.59
```

Commentaire:
convergence detected

Commentaire:
good agreement with the first substructure map obtained in trial 1

```
You can obtain more information about the reconstructed reflection phases by
using 'expandedlog yes'.

Properties of the saved densities:
  Nr. Run  Rvalue   Peaks  Symm.    Der.SG
   1   1   54.21   12.04   9.59        C2
   2   2   54.79    5.70  89.07        Cm
   3   3   55.45    5.32  89.88        Cm
   4   4   55.05    7.50  76.72        Cm
   5   5   56.52   10.61  82.23        Cm
   6   6   54.11   10.36   9.86        C2
   7   7   54.23   11.37  11.59        C2

Current density added to the averaged density. Number of averaged densities:   3

Run number  7. Still  3 to go.


#############
# Iteration #
#############

Estimated delta:  0.0004
Random seed:     123952176

Current k_ed =    1.20000  (absolute delta =   0.00054)
   10  R: 69.985  Charge:      81.39   Peaks:  1.00  Sym:100.00   Score:    ---
   20  R: 69.643  Charge:      79.07   Peaks:  1.13  Sym:100.00   Score:    ---
   30  R: 69.918  Charge:      77.62   Peaks:  1.22  Sym:100.00   Score:    ---
   40  R: 69.887  Charge:      78.03   Peaks:  1.28  Sym:100.00   Score:    ---
   50  R: 69.771  Charge:      76.40   Peaks:  1.35  Sym: 97.46   Score:    ---
   60  R: 70.107  Charge:      75.51   Peaks:  1.35  Sym: 97.46   Score:    ---
   70  R: 69.898  Charge:      76.89   Peaks:  1.40  Sym: 97.46   Score:    ---
   80  R: 70.022  Charge:      76.79   Peaks:  1.43  Sym: 97.46   Score:    ---
   90  R: 70.491  Charge:      75.97   Peaks:  1.50  Sym: 97.46   Score:    ---
  100  R: 70.477  Charge:      74.83   Peaks:  1.45  Sym: 95.77   Score:    ---
  200  R: 70.539  Charge:      74.98   Peaks:  1.67  Sym: 93.28   Score:    ---
  300  R: 70.958  Charge:      74.09   Peaks:  1.74  Sym: 92.94   Score:    ---
  400  R: 70.707  Charge:      73.01   Peaks:  1.91  Sym: 91.75   Score:    ---
  500  R: 70.718  Charge:      72.78   Peaks:  1.96  Sym: 94.32   Score:    ---
  600  R: 70.554  Charge:      73.10   Peaks:  2.11  Sym: 96.00   Score:    ---
  700  R: 70.821  Charge:      71.77   Peaks:  2.11  Sym: 95.92   Score:    ---
  800  R: 70.667  Charge:      71.78   Peaks:  2.25  Sym: 96.65   Score:    ---
  900  R: 70.971  Charge:      72.39   Peaks:  2.10  Sym: 95.06   Score:    ---
 1000  R: 70.657  Charge:      72.25   Peaks:  2.09  Sym: 96.84   Score:    ---
 2000  R: 71.024  Charge:      71.85   Peaks:  2.15  Sym: 94.68   Score:    ---

Calculation is finished. No convergence was detected after  2000 cycles.
Last iteration record:
 2000  R: 71.024  Charge:      71.85   Peaks:  2.15  Sym: 94.68   Score:    ---

    50 cycles of noise suppression follow:
   10  R: 54.907  Charge:       0.00   Peaks:  4.94
   20  R: 55.079  Charge:       0.00   Peaks:  5.70
   30  R: 55.175  Charge:       0.00   Peaks:  6.09
   40  R: 55.173  Charge:       0.00   Peaks:  6.31
   50  R: 55.162  Charge:       0.00   Peaks:  6.50
The density was aligned with the reference file, agreement   69.95%.
Shift:   0.32298  0.13137  0.49328
```

```
####################################
# Checking the density for symmetry #
####################################

Centering vectors:
  0.000  0.000  0.000
  0.500  0.500  0.000

Symmetry operations compatible with the lattice and centering:
                        Symmetry operation            agreement factor
      m(0,1,0):           x1         -x2          x3   10.596    xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
      2(0,1,0):          -x1          x2         -x3   85.196    xxxxxxx
           -1:           -x1         -x2         -x3   85.533    xxxxxxx
      c(0,1,0):           x1         -x2       1/2+x3   97.320    x

-------------------------------------------------
Space group derived from the symmetry operations:
-------------------------------------------------
    HM symbol:     Cm
    Hall symbol:   c -2y
    Fingerprint:   33121063}20 (0,0,0)
    Centering vectors:
      0.000  0.000  0.000
      0.500  0.500  0.000
    Symmetry operations:
               1:            x1           x2           x3
        m(0,1,0):            x1          -x2           x3


#########################################
# Search for the origin of the space group #
#########################################


Position of the origin in the CF map:
  0.0115  0.0000  0.8270
Agreement factors of individual generators:
Number smb agreement
   2   2       85.20

Overall agreement factor:  85.20

You can obtain more information about the reconstructed reflection phases by
using 'expandedlog yes'.

Properties of the saved densities:
  Nr. Run  Rvalue   Peaks  Symm.    Der.SG
   1   1   54.21   12.04    9.59        C2
   2   2   54.79    5.70   89.07        Cm
   3   3   55.45    5.32   89.88        Cm
   4   4   55.05    7.50   76.72        Cm
   5   5   56.52   10.61   82.23        Cm
   6   6   54.11   10.36    9.86        C2
   7   7   54.23   11.37   11.59        C2
   8   8   55.16    6.50   85.20        Cm

Run number  8. Still  2 to go.
```

```
#############
# Iteration #
#############

Estimated delta:  0.0004
Random seed:     124036256

Current k_ed =    1.20000  (absolute delta =   0.00054)
   10  R: 70.016  Charge:      80.22   Peaks:  1.00  Sym:100.00   Score:    ---
   20  R: 70.017  Charge:      79.57   Peaks:  1.10  Sym:100.00   Score:    ---
   30  R: 69.746  Charge:      78.36   Peaks:  1.17  Sym:100.00   Score:    ---
   40  R: 69.544  Charge:      76.99   Peaks:  1.29  Sym:100.00   Score:    ---
   50  R: 69.654  Charge:      75.07   Peaks:  1.41  Sym: 96.21   Score:    ---
   60  R: 69.771  Charge:      76.15   Peaks:  1.37  Sym: 96.21   Score:    ---
   70  R: 70.228  Charge:      75.87   Peaks:  1.42  Sym: 96.21   Score:    ---
   80  R: 70.391  Charge:      75.89   Peaks:  1.44  Sym: 96.21   Score:    ---
   90  R: 70.084  Charge:      75.69   Peaks:  1.49  Sym: 96.21   Score:    ---
  100  R: 70.009  Charge:      75.98   Peaks:  1.51  Sym: 97.14   Score:    ---
  200  R: 70.598  Charge:      74.65   Peaks:  1.67  Sym: 94.07   Score:    ---
  300  R: 70.702  Charge:      73.72   Peaks:  1.91  Sym: 95.30   Score:    ---
  400  R: 70.786  Charge:      73.78   Peaks:  2.02  Sym: 95.26   Score:    ---
  500  R: 70.764  Charge:      73.76   Peaks:  1.92  Sym: 92.46   Score:    ---
  600  R: 70.388  Charge:      72.90   Peaks:  2.14  Sym: 89.39   Score:    ---
  700  R: 71.233  Charge:      71.07   Peaks:  2.46  Sym: 81.15   Score:    ---

Calculation successfully converged after   750 cycles.
Last iteration record:
  750  R: 71.017  Charge:      70.98   Peaks:  2.45  Sym: 81.15   Score:    ---

    50 cycles of noise suppression follow:
   10  R: 53.899  Charge:       0.00   Peaks:  8.06
   20  R: 54.067  Charge:       0.00   Peaks:  9.40
   30  R: 54.197  Charge:       0.00   Peaks:  9.95
   40  R: 54.247  Charge:       0.00   Peaks: 10.19
   50  R: 54.203  Charge:       0.00   Peaks: 10.32
The density was aligned with the reference file, agreement    5.26%.
Shift:   0.67508  0.43218  0.72471


####################################
# Checking the density for symmetry #
####################################

Centering vectors:
  0.000  0.000  0.000
  0.500  0.500  0.000

Symmetry operations compatible with the lattice and centering:
                      Symmetry operation            agreement factor
      2(0,1,0):          -x1          x2          -x3    9.535    xxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
           -1:           -x1          -x2          -x3   78.193    xxxxxxxxxx
      m(0,1,0):           x1          -x2           x3   80.691    xxxxxxxxx
      c(0,1,0):           x1          -x2       1/2+x3   99.185    x

-------------------------------------------------
Space group derived from the symmetry operations:
-------------------------------------------------
    HM symbol:     C2
    Hall symbol:   c 2y
    Fingerprint:   33121060qW0 (0,0,0)
    Centering vectors:
```

```
      0.000  0.000  0.000
      0.500  0.500  0.000
    Symmetry operations:
              1:            x1           x2           x3
        2(0,1,0):           -x1           x2          -x3


##########################################
# Search for the origin of the space group #
##########################################


Position of the origin in the CF map:
  0.0000  0.0000  0.0000
Agreement factors of individual generators:
Number smb agreement
   2   2        9.54

Overall agreement factor:   9.54

You can obtain more information about the reconstructed reflection phases by
using 'expandedlog yes'.

Properties of the saved densities:
  Nr. Run  Rvalue   Peaks  Symm.    Der.SG
   1   1   54.21   12.04   9.59        C2
   2   2   54.79    5.70  89.07        Cm
   3   3   55.45    5.32  89.88        Cm
   4   4   55.05    7.50  76.72        Cm
   5   5   56.52   10.61  82.23        Cm
   6   6   54.11   10.36   9.86        C2
   7   7   54.23   11.37  11.59        C2
   8   8   55.16    6.50  85.20        Cm
   9   9   54.20   10.32   9.54        C2

Current density added to the averaged density. Number of averaged densities:   4

Run number  9. Still  1 to go.


#############
# Iteration #
#############

Estimated delta:  0.0004
Random seed:     124055688

Current k_ed =    1.20000  (absolute delta =   0.00054)
   10  R: 69.910  Charge:      80.18   Peaks:  1.00  Sym:100.00   Score:    ---
   20  R: 69.823  Charge:      78.41   Peaks:  1.12  Sym:100.00   Score:    ---
   30  R: 70.216  Charge:      78.48   Peaks:  1.26  Sym:100.00   Score:    ---
   40  R: 70.088  Charge:      76.65   Peaks:  1.29  Sym:100.00   Score:    ---
   50  R: 70.031  Charge:      77.47   Peaks:  1.30  Sym: 97.79   Score:    ---
   60  R: 70.232  Charge:      76.20   Peaks:  1.36  Sym: 97.79   Score:    ---
   70  R: 70.424  Charge:      76.75   Peaks:  1.38  Sym: 97.79   Score:    ---
   80  R: 69.778  Charge:      77.23   Peaks:  1.37  Sym: 97.79   Score:    ---
   90  R: 70.070  Charge:      75.84   Peaks:  1.43  Sym: 97.79   Score:    ---
  100  R: 69.958  Charge:      76.27   Peaks:  1.40  Sym: 96.89   Score:    ---
  200  R: 70.350  Charge:      75.02   Peaks:  1.68  Sym: 95.72   Score:    ---
  300  R: 70.016  Charge:      73.04   Peaks:  1.98  Sym: 97.26   Score:    ---
```

```
  400  R: 70.866  Charge:      72.43   Peaks:  2.11  Sym: 95.43   Score:    ---
  500  R: 71.241  Charge:      71.88   Peaks:  2.08  Sym: 96.04   Score:    ---
  600  R: 71.086  Charge:      71.40   Peaks:  2.09  Sym: 96.05   Score:    ---
  700  R: 70.533  Charge:      72.49   Peaks:  2.12  Sym: 96.72   Score:    ---
  800  R: 70.868  Charge:      72.03   Peaks:  2.10  Sym: 94.71   Score:    ---
  900  R: 70.930  Charge:      71.71   Peaks:  2.17  Sym: 96.69   Score:    ---
 1000  R: 70.628  Charge:      71.28   Peaks:  2.14  Sym: 95.32   Score:    ---
 2000  R: 71.051  Charge:      72.09   Peaks:  2.15  Sym: 95.76   Score:    ---

Calculation is finished. No convergence was detected after  2000 cycles.
Last iteration record:
 2000  R: 71.051  Charge:      72.09   Peaks:  2.15  Sym: 95.76   Score:    ---

    50 cycles of noise suppression follow:
   10  R: 54.712  Charge:       0.00   Peaks:  4.62
   20  R: 54.616  Charge:       0.00   Peaks:  5.24
   30  R: 54.681  Charge:       0.00   Peaks:  5.63
   40  R: 54.670  Charge:       0.00   Peaks:  5.95
   50  R: 54.650  Charge:       0.00   Peaks:  6.22
The density was aligned with the reference file, agreement   72.48%.
Shift:   0.20661  0.98306  0.60598


####################################
# Checking the density for symmetry #
####################################

Centering vectors:
  0.000  0.000  0.000
  0.500  0.500  0.000

Symmetry operations compatible with the lattice and centering:
                          Symmetry operation             agreement factor
       m(0,1,0):            x1          -x2           x3   12.086
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
       2(0,1,0):           -x1           x2          -x3   89.621    XXX
            -1:            -x1          -x2          -x3   90.283    XXX
       c(0,1,0):            x1          -x2       1/2+x3   96.898    XX

-------------------------------------------------
Space group derived from the symmetry operations:
-------------------------------------------------
    HM symbol:     Cm
    Hall symbol:   c -2y
    Fingerprint:   33121063}20 (0,0,0)
    Centering vectors:
      0.000  0.000  0.000
      0.500  0.500  0.000
    Symmetry operations:
              1:            x1           x2           x3
       m(0,1,0):            x1          -x2           x3


#########################################
# Search for the origin of the space group #
#########################################


Position of the origin in the CF map:
  0.1366  0.0000  0.9196
```

```
Agreement factors of individual generators:
Number smb agreement
   2   2       89.62

Overall agreement factor:  89.62

You can obtain more information about the reconstructed reflection phases by
using 'expandedlog yes'.

Properties of the saved densities:
  Nr. Run  Rvalue   Peaks  Symm.    Der.SG
   1   1   54.21   12.04   9.59        C2
   2   2   54.79    5.70  89.07        Cm
   3   3   55.45    5.32  89.88        Cm
   4   4   55.05    7.50  76.72        Cm
   5   5   56.52   10.61  82.23        Cm
   6   6   54.11   10.36   9.86        C2
   7   7   54.23   11.37  11.59        C2
   8   8   55.16    6.50  85.20        Cm
   9   9   54.20   10.32   9.54        C2
  10  10   54.65    6.22  89.62        Cm

Last run from 10 completed.

Summary of all runs:
Number of attempts          :     10
Maximum cycles              :   2000
Number of successes         :      4
Success rate [%]            :   40.0
Mean cycles per convergence(beta):   3488
95% confidence interval for beta :   1591 -   12800
95% confidence interval for SR   : 0.14 -  0.72

-------------------------------------------
End of the calculation: 19.FEB 2013, 12:41:38
-------------------------------------------
Superflip version: 09/05/11 14:22
```

Commentaire:
best0xx_4F7O.map

Commentaire:
successful trials are 1, 6, 7 and 9.
The derived SG is correct and the symmetry score significant < 10

The corresponding substructure density map are best01-CSN5, best06-CSN5 and best09-CSN5.map

The CSN5.map file corresponding to the average of the best01, best06 and best09 maps is then used for heavy atom sites localization by peak picking.

If necessary, automatic peak-picking on single trial map:
flipsub SG=5 best01_CSN5.map