Supporting Information for:

A detailed example of the identification and crystallographic analysis of a pseudo-merohedrally twinned crystal

Ilia Guzei[a]*, Regine Herbst-Irmer[b], Apollinaire Munyaneza[c] and James Darkwa[d]

[a]Chemistry, University of Wisconsin-Madison, 1101 University Ave., Madison, WI, 53558, USA, [b]Structural Chemistry, University of Goettingen, Tammannstrasse 4, D-37077 Goettingen, Germany, [c]Chemistry, University of Botswana, Private Bag UB00704, Gaborone, Botswana, and [d]Chemistry, University of Johannesburg, Auckland Park Kingsway Campus, PO Box 524, Johannesburg, South Africa

The output from Program XPREP.

Once it was decided the structure was C-centered monoclinic, the data were integrated accordingly and this is the XPREP output similar to the one in Table 2 in the body of the manuscript.

Comments on the way XPREP was run in this case.
To generate the second "`Search for higher metric symmetry`" table both with the orthorhombic and with several monoclinic unit cells the *tolerances* had to be adjusted. Namely, the threshold value (in degrees) for the termination of monoclinic cell searches was changed from the default value of 0.05° to zero. From the main menu select [T] and then select [T] again to make this change. XPREP, thus, is forced to offer more monoclinic unit cell choices. The *I*-centered monoclinic cell is printed only when it has the beta angle closer to 90° compared to the (standard) *C*-centered cell.
The FOM (figure of merit) in the "`Search for higher metric symmetry`" table is the maximum deviation in degrees of a lattice two-fold axis from its expected position.

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
+  XPREP - Reciprocal space exploration - Version 2012/1 for Windows  +
+  Copyright(C) 2012 Bruker-AXS                 All Rights Reserved  +
+  test                           started at 10:22:28 on 10-Jan-2012  +
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++


Original cell in Angstroms and degrees:

   15.218   22.007   16.000    90.00   118.39    90.00

   35930 Reflections read from file test.hkl; mean (I/sigma) =   16.63


Lattice exceptions:  P      A      B      C      I      F     Obv    Rev    All

N (total) =           0  17997  17997      0  17936  17997  23967  23922  35930
N (int>3sigma) =      0  16605  16605      0  16533  16605  22637  22528  33840
Mean intensity =    0.0   21.7   21.7    0.0   21.6   21.7   22.5   21.9   21.9
Mean int/sigma =    0.0   16.4   16.4    0.0   16.4   16.4   16.8   16.5   16.6

Lattice type: C chosen          Volume:      4714.04

-------------------------------------------------------------------------------

DETERMINATION OF REDUCED (NIGGLI) CELL
```

```
Transformation from original cell (HKLF-matrix):
   -0.5000 -0.5000  0.0000   -0.5000  0.5000  0.0000    0.0000  0.0000 -1.0000

Unitcell:      13.378   13.378   16.000  105.69  105.69  110.67

Niggli form:     a.a =    178.97      b.b =    178.97      c.c =    256.01
                 b.c =    -57.89      a.c =    -57.89      a.b =    -63.18

------------------------------------------------------------------------------

Search for higher metric symmetry
Identical indices and Friedel opposites combined before calculating R(sym)
------------------------------------------------------------------------------
Option A: FOM = 0.005 deg.   ORTHORHOMBIC F-lattice   R(sym) = 0.044 [   6070]
Cell:   15.218  22.007  28.152   90.00   90.00   90.00    Volume:      9428.08
Matrix:-1.0000  0.0000  0.0000  0.0000  1.0000  0.0000 -1.0000  0.0000 -2.0000

Option A selected

------------------------------------------------------------------------------

SPACE GROUP DETERMINATION


Lattice exceptions:  P      A      B      C      I      F     Obv    Rev    All

N (total) =           0      0      0      0  17951      0  23947  23922  35930
N (int>3sigma) =      0      0      0      0  17318      0  22573  22528  33840
Mean intensity =    0.0    0.0    0.0    0.0   22.3    0.0   22.0   21.9   21.9
Mean int/sigma =    0.0    0.0    0.0    0.0   17.4    0.0   16.6   16.5   16.6


Crystal system O and Lattice type F selected

Mean |E*E-1| = 0.603 [expected .968 centrosym and .736 non-centrosym]

Chiral flag NOT set



Systematic absence exceptions:

         d--   -d-   --d

N       740   598   471
N I>3s  588     1   396
<I>     8.7   0.2  24.7
<I/s>  11.0   0.6  14.9


Identical indices and Friedel opposites combined before calculating R(sym)
```

```
Option  Space Group  No.  Type  Axes  CSD  R(sym) N(eq)  Syst. Abs.   CFOM

No acceptable space group -  change tolerances or unset chiral flag
or possibly change input lattice type, then recheck cell using H-option


------------------------------------------------------------------------------

TOLERANCES CHANGED

Maximum deviation (deg.) in higher symmetry cell search =  1.000
Threshold (deg.) for terminating search =  0.000
R(int) maximum for terminating cell search =  0.120
R(int) maximum for space group determination =  0.300
Minimum number of data in group for syst. absence test =   5
Maximum mean I/sigma(I) for systematic absences =  3.163
Minimum I/sigma gap between absences and rest =  3.326

------------------------------------------------------------------------------

DETERMINATION OF REDUCED (NIGGLI) CELL

Transformation from original cell (HKLF-matrix):
   -0.5000 -0.5000  0.0000   -0.5000  0.5000  0.0000    0.0000  0.0000 -1.0000

Unitcell:      13.378   13.378   16.000  105.69  105.69  110.67

Niggli form:     a.a =    178.97      b.b =    178.97      c.c =    256.01
                 b.c =    -57.89      a.c =    -57.89      a.b =    -63.18

------------------------------------------------------------------------------

Search for higher metric symmetry
Identical indices and Friedel opposites combined before calculating R(sym)
------------------------------------------------------------------------------
Option A: FOM = 0.005 deg.   ORTHORHOMBIC F-lattice   R(sym) = 0.044 [   6070]
Cell:   15.218  22.007  28.152   90.00   90.00   90.00    Volume:      9428.08
Matrix:-1.0000  0.0000  0.0000  0.0000  1.0000  0.0000 -1.0000  0.0000 -2.0000
------------------------------------------------------------------------------
Option B: FOM = 0.000 deg.   MONOCLINIC   C-lattice   R(sym) = 0.024 [   3920]
Cell:   15.218  22.007  16.000   90.00  118.39   90.00    Volume:      4714.04
Matrix: 1.0000  0.0000  0.0000  0.0000  1.0000  0.0000  0.0000  0.0000  1.0000
------------------------------------------------------------------------------
Option C: FOM = 0.005 deg.   MONOCLINIC   C-lattice   R(sym) = 0.039 [   3997]
Cell:   22.007  15.218  17.866   90.00  128.02   90.00    Volume:      4714.04
Matrix: 0.0000  1.0000  0.0000  1.0000  0.0000  0.0000 -0.5000 -0.5000 -1.0000
------------------------------------------------------------------------------
Option D: FOM = 0.005 deg.   MONOCLINIC   I-lattice   R(sym) = 0.039 [   3997]
Cell:   17.866  15.218  17.866   90.00  103.97   90.00    Volume:      4714.04
Matrix: 0.5000  0.5000  1.0000  1.0000  0.0000  0.0000 -0.5000  0.5000 -1.0000
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Option E: FOM = 0.005 deg.   MONOCLINIC   C-lattice   R(sym) = 0.044 [   3957]
Cell:   15.218  28.152  13.378   90.00  124.66   90.00    Volume:      4714.04
Matrix: 1.0000  0.0000  0.0000  1.0000  0.0000  2.0000 -0.5000 -0.5000  0.0000
--------------------------------------------------------------------------------
Option F: FOM = 0.005 deg.   MONOCLINIC   I-lattice   R(sym) = 0.044 [   3957]
Cell:   13.378  28.152  13.378   90.00  110.67   90.00    Volume:      4714.04
Matrix: 0.5000  0.5000  0.0000  1.0000  0.0000  2.0000  0.5000 -0.5000  0.0000
--------------------------------------------------------------------------------
Option G: FOM = 0.000 deg.   TRICLINIC    P-lattice   R(sym) = 0.000 [      0]
Cell:   13.378  13.378  16.000  105.69  105.69  110.67    Volume:      2357.02
Matrix:-0.5000 -0.5000  0.0000 -0.5000  0.5000  0.0000  0.0000  0.0000 -1.0000

Option B selected

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SPACE GROUP DETERMINATION


Lattice exceptions:  P      A      B      C      I      F     Obv    Rev    All

N (total) =          0  17997  17997      0  17936  17997  23967  23922  35930
N (int>3sigma) =     0  16605  16605      0  16533  16605  22637  22528  33840
Mean intensity =   0.0   21.7   21.7    0.0   21.6   21.7   22.5   21.9   21.9
Mean int/sigma =   0.0   16.4   16.4    0.0   16.4   16.4   16.8   16.5   16.6


Crystal system M and Lattice type C selected

Mean |E*E-1| = 0.615 [expected .968 centrosym and .736 non-centrosym]

Chiral flag NOT set



Systematic absence exceptions:

         -c-

N       598
N I>3s    1
<I>     0.2
<I/s>   0.6


Identical indices and Friedel opposites combined before calculating R(sym)

Option  Space Group  No.  Type  Axes  CSD  R(sym) N(eq)  Syst. Abs.   CFOM

[A] C2/c           # 15  centro   1  3696  0.024   3920  0.6 / 16.6  13.13
```

[B] Cc   # 9 non-cen 1   566 0.024   3920 0.6 / 16.6   2.27

Option [B] chosen

INTENSITY STATISTICS FOR DATASET # 1 test.hkl

Resolution	#Data	#Theory	%Complete	Redundancy	Mean I	Mean I/s	Rmerge	Rsigma
Inf - 3.48	126	131	96.2	5.75	103.0	88.86	0.0157	0.0102
3.48 - 2.33	288	293	98.3	6.81	56.9	82.29	0.0192	0.0112
2.33 - 1.84	419	423	99.1	7.13	45.5	69.81	0.0233	0.0128
1.84 - 1.60	424	427	99.3	6.70	44.3	64.59	0.0233	0.0140
1.60 - 1.45	419	423	99.1	6.36	26.0	46.00	0.0324	0.0187
1.45 - 1.35	391	393	99.5	5.51	18.3	34.09	0.0400	0.0249
1.35 - 1.27	427	436	97.9	4.62	16.6	33.34	0.0413	0.0279
1.27 - 1.20	429	459	93.5	5.20	16.2	35.53	0.0425	0.0278
1.20 - 1.15	372	394	94.4	4.92	13.4	29.56	0.0456	0.0326
1.15 - 1.10	433	471	91.9	4.69	12.2	28.17	0.0491	0.0353
1.10 - 1.06	433	462	93.7	4.22	9.5	22.93	0.0519	0.0428
1.06 - 1.02	465	502	92.6	3.91	10.1	23.56	0.0516	0.0432
1.02 - 0.99	433	459	94.3	3.66	9.1	21.62	0.0540	0.0463
0.99 - 0.96	440	500	88.0	3.25	7.6	19.39	0.0586	0.0518
0.96 - 0.94	283	334	84.7	2.59	7.6	17.77	0.0576	0.0553
0.94 - 0.91	543	661	82.1	2.58	6.0	16.28	0.0639	0.0611
0.91 - 0.89	342	414	82.6	2.23	5.3	14.71	0.0652	0.0669
0.89 - 0.87	410	538	76.2	1.94	5.2	15.18	0.0622	0.0658
0.87 - 0.85	430	542	79.3	1.76	4.3	13.00	0.0643	0.0749
0.85 - 0.83	444	625	71.0	1.32	3.7	11.69	0.0603	0.0820
0.83 - 0.81	278	656	42.4	0.57	3.3	10.05	0.0676	0.0893
0.91 - 0.81	1904	2775	68.6	1.48	4.4	13.04	0.0634	0.0738
Inf - 0.81	8229	9543	86.2	3.77	16.9	30.90	0.0309	0.0259

Merged [S], lowest resolution = 14.08 Angstroms

Current dataset is # 1 test.hkl

Determination of unit-cell contents

Formula: C44 H42 Br5 Fe3 N6 Ni O4

Formula weight =   1344.59

Tentative Z (number of formula units/cell) =   4.0 giving rho = 1.895,
non-H atomic volume = 18.7 and following cell contents and analysis:

```
 C     176.00    39.30 %              H     168.00     3.15 %
 N      24.00     6.25 %              O      16.00     4.76 %
 Fe     12.00    12.46 %              Ni      4.00     4.37 %
 Br     20.00    29.71 %

F(000) =    2644.0        Cu-K(alpha) radiation        Mu (mm-1) =  13.07


--------------------------------------------------------------------------------

File test.ins set up as follows:

TITL test in Cc
CELL 1.54178  15.2180  22.0068  16.0004  90.000 118.391  90.000
ZERR    4.00   0.0003   0.0004   0.0003   0.000   0.001   0.000
LATT -7
SYMM X, -Y, 0.5+Z
SFAC C H N O FE NI BR
UNIT 176 168 24 16 12 4 20
TEMP -173.140
TREF
HKLF 4
END

   35930 Reflections written to new reflection file test.hkl

--------------------------------------------------------------------------------
```

The output from Program PLATON that tested the diffraction data for twinning.
The twin law used is highlighted in red.

```
                                                                                                                "test      "  PLATON-GENERAL   Page    1
=============================================================================================================================================
PLATON(V-150911)-Run for: test                   R = 0.17                                                          TIME: Jan 10 10:37:08 2012
=============================================================================================================================================
                                                                                                                                (C) 1980-2011 A.L.Spek
                                                    ============
================================================== Crystal Data ================================================================================
                                                    ============
                        Input Cell  (Lattice Type: C)   -   Temp = 100K            Reduced Cell     (Acta Cryst.(1976),A32,297-298)
-------------------------------------------------------------------------------   ---------------------------------------------
a =    15.2180(3)  Angstrom               alpha =           90 Degree             a  =   13.378     alpha  =  105.69  V  =  2357.0
b =    22.0068(4)                          beta =    118.391(1)                   b  =   13.378     beta   =  105.69
c =    16.0004(3)                         gamma =           90                    c  =   16.000     gamma  =  110.67

V =   4714.02(16) Cubic-Angstrom         d(100) =     13.3876   Angstrom                    Niggli Values
                                         d(010) =     22.0068                       178.972   178.972   256.013
Lambda(CuKa) =   1.54178 Angstrom        d(001) =     14.0759                       -57.889   -57.889   -63.178

                                              ==========================
============================================== Orthogonalization Matrices ==================================================================
                                              ==========================

(See e.g. J.D.Dunitz, Xray Analysis and Structure Determination of Organic Molecules, Cornell Univ. Press, 1979, P236)

(XO)   (  15.21800         0  -7.60797 ) (X)   ,   (X)   (   0.06571         0   0.03552 ) (XO)      Orthogonal Axes AO, BO and CO
(YO) = (         0  22.00680         0 )*(Y)   ,   (Y) = (         0   0.04544         0 )*(YO)            are defined as:
(ZO)   (         0         0  14.07592 ) (Z)   ,   (Z)   (         0         0   0.07104 ) (ZO)     AO // A, CO // C*, BO // CO X AO

                                               ====================
================================================ Space Group Symmetry ==========================================================
                                               ====================

(See e.g. G. Burns & A.M. Glazer, Space Groups for Solid State Scientists, Academic Press, 1990 or Int. Tables A)

Space Group Cc                     No:   9, Laue:  2/m [Hall:  C -2yc          ]

Lattice Type mC, Acentric,   Monoclinic, Order   4( 2) [Schoenflies: Cs^4      ]

ACHIRAL - See P.G. Jones, Acta Cryst. (1986), A42, 57.

  Nr            ***** Symmetry Operation(s) *****

   1              X ,             Y ,             Z
   2              X ,           - Y ,       1/2 + Z
```

```
3        1/2 + X ,       1/2 + Y ,             Z
4        1/2 + X ,       1/2 - Y ,       1/2 + Z
```

(1:19-Rule Rounded) Coordinates of Unique Residue(s) Identified. Standard Deviations in the Last Digit are in Parentheses.

```
         Site    = Site Symmetry; SSN = Site Symmetry Number; SSOF = SHELX Site Occupation Factor (= S.O.F / SSN).
*******  Move    = Transformation on Input Data: N.IJK (N = SymOp, IJK = Translation) i.e. 1.555 = nomove
SYMBOLS: Type    = D/A = Potential Donor or Acceptor atom, D-H = H on Donor atom, MET = Metal.
*******  El Type = AK = Alkali Metal, AE = Alkaline Earth, HL = Halogen, AN = Actinide, LN = Lanthanide, TR = Transition Element.
         ARU     = Asymmetric Residue Unit encoded as sklm.nn, with s = symmetry op, klm = translation, nn = residue #.
         RESIDUE = collection of ARU's constituting an isolated unit (= molecule, ion).
         FLAGS   : d = determined, c = calculated, R = riding G = group
```

Atom Types :	C	Br	Fe	N	Ni	O
Cov.Rad(Ang):	0.68	1.21	1.45	0.68	1.50	0.68
Atom Volume :	13.87	32.70	30.40	11.80	26.00	11.39
Atom Number :	6	35	26	7	28	8
Atom Weight :	12.010	79.900	55.85	14.01	58.69	16.00
Scat.Fact.f0:	5.999	34.993	25.990	6.995	27.988	7.999
Scat.Fact.f':	0.018	-0.676	-1.134	0.031	-3.003	0.049
Scat.Fact.f":	0.009	1.281	3.197	0.018	0.509	0.032
Mu/Rho(CuKa):	4.51	88.94	301.92	7.44	48.84	11.44
Elem. Type :	--	HL	TR	--	TR	--

Sources - Cov. Radii : Manual Cambridge Crystallographic Data Base
- Atom Volume: D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493
- Atomic Wt. : SHELXL97 NOMOVE
- Scat. Fact.: SHELXL97 (International Tables)
- mu/rho : International Tables C, table 4.2.4.2, p193-199

Residue = 1

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN*SSOF =	S.O.F	Move	Type
d	Br(1)	0.26801(18)	0.12267(11)	0.42705(17)	0.830(3)	2.700(2)	6.011(2)	1	1	1	-	D/A
d	Ni(2)	0.1814(3)	0.12432(16)	0.2538(3)	0.830(5)	2.736(4)	3.572(4)	1	1	1	-	Met
d	Fe(5)	0.5617(3)	0.17601(17)	0.3581(3)	5.824(5)	3.873(4)	5.041(4)	1	1	1	-	Met
d	Fe(6)	-0.0944(3)	0.07857(17)	0.3560(3)	-4.145(5)	1.729(4)	5.011(4)	1	1	1	-	Met
d	O(1)	0.2685(19)	0.4093(11)	0.2015(19)	2.55(3)	9.01(2)	2.84(3)	1	1	1	-	D/A
d	O(3)	0.1322(15)	0.3730(8)	0.1847(15)	0.61(3)	8.209(18)	2.60(2)	1	1	1	-	D/A
d	O(4)	0.0347(17)	-0.1586(10)	0.2104(17)	-1.07(3)	-3.49(2)	2.96(2)	1	1	1	-	D/A
d	O(9)	0.1625(14)	-0.1357(8)	0.2008(14)	0.95(2)	-2.986(18)	2.83(2)	1	1	1	-	D/A
d	N(1I)	0.1049(13)	0.0448(8)	0.2524(13)	-0.32(2)	0.986(18)	3.553(18)	1	1	1	-	D/A
d	N(2)	0.2068(15)	0.2624(9)	0.2416(15)	1.31(3)	5.77(2)	3.40(2)	1	1	1	-	D/A
d	N(4)	0.2576(15)	0.2078(9)	0.2597(15)	1.94(3)	4.57(2)	3.66(2)	1	1	1	-	D/A
d	N(5)	0.0540(13)	0.1630(8)	0.1543(13)	-0.35(2)	3.587(18)	2.172(18)	1	1	1	-	D/A
d	N(8)	0.2131(12)	0.0868(7)	0.1510(12)	2.09(2)	1.910(15)	2.125(17)	1	1	1	-	D/A
d	N(14)	0.1463(14)	-0.0079(9)	0.2417(14)	0.39(2)	-0.17(2)	3.40(2)	1	1	1	-	D/A

d	C(1)	-0.167(3)	0.0522(15)	0.427(3)	-5.79(5)	1.15(3)	6.01(4)	1	1	1	-	-
d	C(1A)	0.2395(13)	-0.0078(8)	0.2457(13)	1.78(2)	-0.172(18)	3.458(18)	1	1	1	-	-
d	C(1B)	-0.0472(14)	0.0758(8)	0.2601(14)	-2.70(2)	1.668(18)	3.66(2)	1	1	1	-	-
d	C(1C)	0.0184(17)	0.0322(10)	0.2451(17)	-1.58(3)	0.71(2)	3.45(2)	1	1	1	-	-
d	C(1D)	-0.149(2)	0.0799(13)	0.214(2)	-3.90(3)	1.76(3)	3.01(3)	1	1	1	-	-
d	C(1E)	0.540(3)	0.1307(17)	0.236(3)	6.42(5)	2.88(4)	3.32(4)	1	1	1	-	-
d	C(1F)	0.514(2)	0.0870(12)	0.306(2)	5.49(3)	1.91(3)	4.31(3)	1	1	1	-	-
d	C(1G)	-0.019(2)	0.1305(12)	0.073(2)	-0.84(3)	2.87(3)	1.03(3)	1	1	1	-	-
d	C(1H)	0.3426(18)	0.2203(11)	0.2505(18)	3.31(3)	4.85(2)	3.53(3)	1	1	1	-	-
d	C(1I)	0.191(2)	-0.2036(15)	0.194(2)	1.43(3)	-4.48(3)	2.73(3)	1	1	1	-	-
d	C(1J)	-0.0548(16)	0.2507(10)	0.0852(16)	-1.48(3)	5.52(2)	1.20(2)	1	1	1	-	-
d	C(1K)	-0.016(2)	0.1318(11)	0.317(2)	-2.66(3)	2.90(2)	4.46(3)	1	1	1	-	-
d	C(1L)	0.651(2)	0.2538(13)	0.407(2)	6.81(3)	5.59(3)	5.73(3)	1	1	1	-	-
d	C(1M)	0.3401(17)	0.2811(10)	0.2301(17)	3.43(3)	6.19(2)	3.24(2)	1	1	1	-	-
d	C(1N)	0.6985(16)	0.1988(9)	0.4282(16)	7.37(3)	4.37(2)	6.03(2)	1	1	1	-	-
d	C(1O)	-0.187(2)	0.1272(14)	0.237(2)	-4.65(3)	2.80(3)	3.34(3)	1	1	1	-	-
d	C(1P)	-0.031(2)	-0.0073(15)	0.442(2)	-3.83(3)	-0.16(3)	6.22(3)	1	1	1	-	-
d	C(1Q)	0.609(3)	0.1938(16)	0.502(3)	5.45(5)	4.26(4)	7.07(4)	1	1	1	-	-
d	C(1R)	0.0901(16)	-0.1229(9)	0.2109(16)	-0.23(3)	-2.70(2)	2.97(2)	1	1	1	-	-
d	C(1S)	0.253(3)	0.0285(18)	0.021(3)	3.69(5)	0.63(4)	0.30(4)	1	1	1	-	-
d	C(1T)	-0.087(3)	0.162(2)	-0.010(3)	-1.25(5)	3.57(4)	-0.14(4)	1	1	1	-	-
d	C(1U)	-0.115(2)	0.2172(13)	0.006(2)	-1.80(3)	4.78(3)	0.08(3)	1	1	1	-	-
d	C(2)	0.2519(17)	0.3061(10)	0.2291(17)	2.09(3)	6.74(2)	3.22(2)	1	1	1	-	-
d	C(3)	0.230(2)	0.3667(12)	0.215(2)	1.86(3)	8.07(3)	3.03(3)	1	1	1	-	-
d	C(4)	0.1120(16)	0.2573(10)	0.2448(16)	-0.16(3)	5.66(2)	3.45(2)	1	1	1	-	-
d	C(5)	0.2103(18)	0.1174(11)	0.0861(18)	2.55(3)	2.58(2)	1.21(3)	1	1	1	-	-
d	C(6)	0.0333(15)	0.2228(9)	0.1592(15)	-0.70(3)	4.90(2)	2.24(2)	1	1	1	-	-
d	C(7)	0.253(2)	-0.0018(12)	0.090(2)	3.17(3)	-0.04(3)	1.27(3)	1	1	1	-	-
d	C(8)	0.229(2)	0.0957(12)	0.013(2)	3.39(3)	2.11(3)	0.18(3)	1	1	1	-	-
d	C(9)	0.063(4)	0.427(2)	0.130(4)	-0.03(7)	9.40(4)	1.83(6)	1	1	1	-	-
d	C(10)	0.2323(18)	0.0307(11)	0.1601(19)	2.32(3)	0.68(2)	2.25(3)	1	1	1	-	-
d	C(11)	0.687(2)	0.1630(14)	0.490(2)	6.73(3)	3.59(3)	6.90(3)	1	1	1	-	-
d	C(12)	0.5854(18)	0.2468(11)	0.4475(18)	5.50(3)	5.43(2)	6.30(3)	1	1	1	-	-
d	C(13)	0.432(2)	0.1165(12)	0.313(2)	4.19(3)	2.56(3)	4.41(3)	1	1	1	-	-
d	C(14)	-0.1360(16)	-0.0012(10)	0.3984(17)	-5.10(3)	-0.03(2)	5.61(2)	1	1	1	-	-
d	C(15)	-0.1109(16)	0.1620(9)	0.2960(16)	-3.94(3)	3.57(2)	4.17(2)	1	1	1	-	-
d	C(16)	-0.0013(17)	-0.0278(10)	0.2380(17)	-1.83(3)	-0.61(2)	3.35(2)	1	1	1	-	-
d	C(17)	0.0838(17)	-0.0551(10)	0.2326(17)	-0.49(3)	-1.21(2)	3.27(2)	1	1	1	-	-
d	C(18)	0.4122(19)	0.1743(11)	0.2648(18)	4.26(3)	3.84(2)	3.73(3)	1	1	1	-	-
d	C(19)	0.471(2)	0.1766(12)	0.215(2)	5.53(3)	3.89(3)	3.03(3)	1	1	1	-	-
d	C(20)	-0.082(2)	0.0851(14)	0.494(2)	-5.01(3)	1.87(3)	6.95(3)	1	1	1	-	-
d	C(21)	-0.003(3)	0.0524(16)	0.482(3)	-3.71(5)	1.15(4)	6.78(4)	1	1	1	-	-

Residue = 2

Flags	Label	Fractional Coordinates (x,y,z)			Orthogonal Coordinates (XO,YO,ZO)			Site	SSN*SSOF = S.O.F		Move	Type
dP	>Br(2)	0.4133(4)	-0.1359(2)	0.2396(3)	4.467(7)	-2.991(4)	3.373(4)	1	0.700	0.700(8)	-	D/A
dP	>Br(3)	0.6626(4)	-0.1431(2)	0.4562(3)	6.613(7)	-3.149(4)	6.421(4)	1	0.700	0.700(8)	-	D/A
dP	>Br(4)	0.4745(4)	-0.0288(2)	0.4487(4)	3.807(7)	-0.634(4)	6.316(6)	1	0.700	0.700(8)	-	D/A
dP	>Br(5)	0.4229(4)	-0.1951(2)	0.4642(4)	2.904(7)	-4.294(4)	6.534(6)	1	0.700	0.700(8)	-	D/A
d	Fe(4)	0.5034(4)	-0.1272(2)	0.4049(4)	4.580(7)	-2.799(4)	5.699(6)	1	1	1	-	Met

Disordered Atoms with S.O.F < 0.5

dP	<Br(2A)	0.4387(7)	-0.1153(4)	0.2407(6)	4.845(12)	-2.537(9)	3.388(8)	1	0.300	0.300(8)	-	D/A
dP	<Br(3A)	0.6508(7)	-0.0543(4)	0.4666(7)	6.354(12)	-1.195(9)	6.568(10)	1	0.300	0.300(8)	-	D/A
dP	<Br(4A)	0.4063(7)	-0.1086(4)	0.4593(7)	2.689(12)	-2.390(9)	6.465(10)	1	0.300	0.300(8)	-	D/A
dP	<Br(5A)	0.5875(8)	-0.2196(5)	0.4536(8)	5.490(14)	-4.833(11)	6.385(11)	1	0.300	0.300(8)	-	D/A

NOTE: Atoms preceded by > * or < indicate disordered positions (SOF : < 50%, 50%, > 50%)

Disordered Structure — Unit Cell Contents (Based on Contents of Atom List, that may be Incomplete)

Resd	Site	X(cen)	Y(cen)	Z(cen)	Mol.Wt	S.O.F	Z	C	Br	Fe	N	Ni	O
1	1	0.191	1/8	0.273	902.77	1	4	42	1	2	6	1	4
2	1	0.507	-0.125	0.404	375.45	1	4	-	4	1	-	-	-
					Unit Cell Weight =			5112.88	168	20	12	24	4	16
					Calculated Analysis (%) =				39.5	31.3	13.1	6.6	4.6	5.0

Moiety_Formula = C42 Br Fe2 N6 Ni O4, Br4 Fe

Sum_Formula = C42 Br5 Fe3 N6 Ni O4

Formula_Weight = 1278.22 [Note: Based on SHELXL97 Atomic Weights]

Formula_Z = 4

SpaceGroup_Z = 4 ===> Z' = 4 / 4 = 1.000

Calculated Density = 1.8011(1) g cm-3 [= Mg m-3]

F(000) = 2428.0 [2393.84]

mu(CuKa) = 130.50 cm-1 = 13.050 mm-1

** WARNING **
Please Check the Derived Crystal Data.
They may be Incorrect for Disordered,
Incomplete or Polymeric Structures.

Resonant Scattering = 844 * 0.0001 - (E. Girard et al. (2003). Acta Cryst. D59, 1914-1922)

Friedif = 1113 - (H. Flack & U. Shmueli (2007). Acta Cryst. A63, 257-265)

Predicted Volume = 3918.4[3844.7] Ang**3, 298[100]K - (D.W.M. Hofmann (2002). Acta Cryst. B58, 489-493)

Note on F000: The first number is a pure electron count, the second number between [] is calculated from f,f' & f"

TwinRotMat: Analysis of the Fo/Fc CIF for Unaccounted (Non)Merohedral Twinning

'calc w=1/[\s^2^(Fo^2^)+(0.1000P)^2^] where P=(Fo^2^+2Fc^2^)/3'

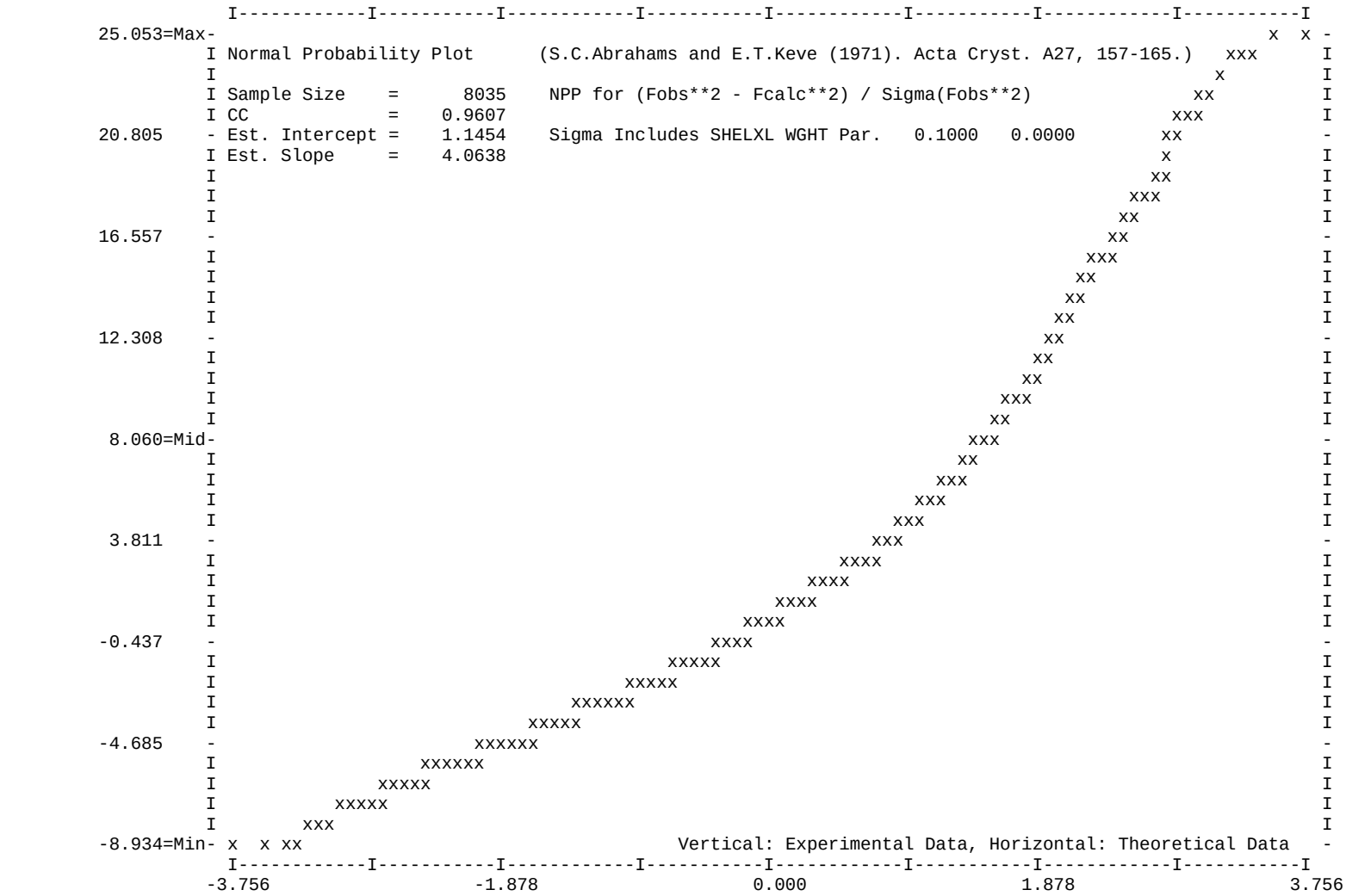
:: Reflection Data are READ from File : test.fcf - (FoFc-Data)

:: Hmax = 18, Kmax = 27, Lmax = 19

:: Sigma Includes SHELXL WGHT Par. 0.1000 0.0000

ST/L	d	#	Nobs	R1	wR2	S	0 Percent Distr. for I .gt. 2*s(I) 100
0.30	1.66	1063	1062	0.145	0.487	5.504	**.
0.38	1.32	1087	1085	0.157	0.455	4.582	**.
0.44	1.15	1031	1027	0.169	0.487	4.880	**.
0.48	1.04	1016	1004	0.178	0.489	4.622	**.
0.52	0.97	1009	999	0.172	0.453	4.114	**.
0.55	0.91	931	917	0.187	0.459	3.943	**.
0.58	0.87	859	828	0.211	0.497	4.078	**..
0.60	0.83	798	754	0.205	0.469	3.477	**...
0.63	0.80	241	230	0.211	0.485	3.294	**..
							I I I
			Percent Observed:				0 50 100

:: R1 = 0.169, wR2 = 0.475, S = 4.454, Nref = 8035, Nobs = 7906, Npar = 262


Normal Probability Plot (S.C.Abrahams and E.T.Keve (1971). Acta Cryst. A27, 157-165.)
Sample Size = 8035 NPP for (Fobs**2 - Fcalc**2) / Sigma(Fobs**2)
CC = 0.9607
Est. Intercept = 1.1454 Sigma Includes SHELXL WGHT Par. 0.1000 0.0000
Est. Slope = 4.0638
Vertical: Experimental Data, Horizontal: Theoretical Data
25.053=Max
20.805
16.557
12.308
8.060=Mid
3.811
-0.437
-4.685
-8.934=Min
-3.756
-1.878
0.000
1.878
3.756

H	K	L	Iobs	Icalc	SigI	Delt/Sig	Theta	DTheta	Alpha	Rot Axis
-2	6	-1	32614.31	4177.87	245.74	115.72	14.94			
-2	4	0	17616.55	2694.54	144.42	103.32	10.45			
-4	4	3	14565.46	2903.23	126.05	92.52	14.62			
-8	4	7	16955.48	822.29	176.09	91.62	27.34			
-3	3	0	11952.37	2051.32	110.31	89.76	11.67			
-2	8	-2	11560.06	603.76	122.99	89.08	19.89			
-5	1	4	19889.26	3048.67	200.21	84.11	15.58			
-4	6	0	24559.67	8136.46	198.61	82.69	18.17			
2	6	1	31222.63	2051.78	357.72	81.55	14.94			
-5	1	3	26387.78	8725.84	217.56	81.18	14.90			
5	1	-4	24350.47	5298.56	237.04	80.37	15.58			
-1	5	-7	17723.93	4419.33	165.85	80.22	26.70			
-1	7	-2	24839.89	8728.69	202.84	79.43	16.58			
-5	3	-1	13425.90	3800.54	130.60	73.70	19.55			
-3	5	-3	17964.87	5547.58	170.65	72.76	19.78			
-1	7	-5	10448.88	980.00	133.30	71.03	23.06			
-1	7	-1	25050.98	10123.12	211.71	70.51	15.28			
2	4	0	13539.84	1208.13	175.07	70.44	10.45			
-1	7	4	7618.12	368.47	103.67	69.93	18.38			
-3	5	0	24474.64	10692.55	198.02	69.60	14.24			
-1	7	-4	22893.90	7712.53	219.05	69.31	20.57			
-9	3	3	28778.91	9029.24	288.76	68.39	28.36			
-4	4	5	34350.73	13772.55	310.43	66.29	17.22			
-2	0	-4	14710.15	2693.87	182.03	66.01	16.98			
2	8	2	10092.63	1073.19	140.27	64.30	19.89			
-2	8	2	20079.67	7659.59	194.79	63.76	17.64			
-5	3	3	8695.55	2503.08	97.28	63.66	16.00			
-2	8	6	10878.49	431.43	170.57	61.25	23.87			
-3	5	-6	9787.20	1256.13	139.60	61.11	28.14			
-6	4	4	7454.67	2041.60	88.70	61.03	19.82			
-2	6	5	21714.31	7246.88	240.17	60.24	18.67			
-4	4	-3	14332.70	5755.31	144.49	59.36	21.61			
1	5	-4	15433.20	4555.42	183.38	59.32	15.34			
-5	1	-3	7710.09	1090.10	112.84	58.67	23.27			
-3	7	1	29856.79	16281.63	236.14	57.49	16.84			
-2	2	-4	19193.25	9957.06	160.98	57.37	17.47			
-6	8	6	13587.78	3359.10	179.04	57.13	26.42			
1	7	-4	9159.87	713.91	148.07	57.04	18.38			
4	6	0	20826.17	3773.33	299.72	56.90	18.17			
0	8	-1	26349.68	11118.59	272.05	55.99	16.59			
1	7	2	19301.51	4247.51	276.11	54.52	16.58			
-3	5	-4	18666.36	9409.40	171.60	53.94	22.34			
-3	1	-2	13664.34	7377.58	116.73	53.86	14.31			
3	3	0	9164.93	1382.78	144.49	53.86	11.67			
0	8	1	26993.18	11241.82	293.18	53.73	16.59			

-3	7	4	8391.39	3333.62	94.40	53.58	18.62
9	3	-3	25776.07	6979.67	354.60	53.01	28.36
1	7	1	24694.37	8664.27	302.87	52.93	15.28
4	4	-3	13579.00	338.42	251.90	52.56	14.62
0	6	0	19120.59	8507.53	214.56	49.46	12.13

Criteria: DeltaI/SigmaI .GT. 4.0, DeltaTheta 0.10 Deg., NselMin = 50

Wavelength Used in this Analysis 1.54178 Ang.

N(refl) = 8035, N(selected) = 50, IndMax = 5, CritI = 0.1, CritT = 0.10

2-axis (0 0 1) [1 0 2], Angle () [] = 0.00 Deg, Freq = 100
****
(-1.000 0.000 0.000) (h1) (h2) Nr Overlap = 8035
(0.000 -1.000 0.000) * (k1) = (k2) BASF = 0.44
(1.000 0.000 1.000) (l1) (l2) DEL-R =-0.038

2-axis (0 1 0) [0 1 0], Angle () [] = 0.00 Deg, Freq = 98
****
(-1.000 0.000 0.000) (h1) (h2) Nr Overlap = 8035
(0.000 1.000 0.000) * (k1) = (k2) BASF = 0.17
(0.000 0.000 -1.000) (l1) (l2) DEL-R =-0.001

2-axis (1 -1 -1) [5 -3 -4], Angle () [] = 2.63 Deg, Freq = 18
****
(-0.200 -0.540 -0.660) (h1) (h2) Nr Overlap = 746
(-0.800 -0.460 0.660) * (k1) = (k2) BASF = 0.05
(-0.800 0.540 -0.340) (l1) (l2) DEL-R =-0.001

2-axis (1 1 -1) [5 3 -4], Angle () [] = 2.63 Deg, Freq = 16
****
(-0.200 0.540 -0.660) (h1) (h2) Nr Overlap = 742
(0.800 -0.460 -0.660) * (k1) = (k2) BASF = 0.06
(-0.800 -0.540 -0.340) (l1) (l2) DEL-R =-0.001

Note: Symmetry Equivalent Twin Laws are not Listed !

:: SPF File on :test.eld