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==================================================================================================================================
PLATON(V-101204)-Run for: EUSE                                                                          TIME: Dec 10 13:35:43 2004
==================================================================================================================================
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(C) 1980-2004 A.L.Spek

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                                                         ============
===================================================== Crystal Data ===============================================================
                                                         ============
                        Input Cell  (Lattice Type: I)   -   Temp =   0K           Reduced Cell     (Acta Cryst.(1976),A32,297-298)
-------------------------------------------------------------------------------   -----------------------------------------------
a =         6.3910  Angstrom                alpha =           90 Degree           a  =    5.985     alpha  =   98.06  V  =   160.3
b =         6.3910                           beta =           90                  b  =    5.985     beta   =  115.46
c =         7.8480                          gamma =           90                  c  =    5.985     gamma  =  115.46

V =         320.55  Cubic-Angstrom         d(100) =      6.3910   Angstrom                   Niggli Values
                                           d(010) =      6.3910                         35.820    35.820    35.820
Lambda(MoKa) =   0.71073 Angstrom          d(001) =      7.8480                         -5.025   -15.398   -15.398

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

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

(XO)   (   6.39100         0         0 ) (X)   ,   (X)   (   0.15647         0         0 ) (XO)      Orthogonal Axes AO, BO and CO
(YO) = (         0   6.39100         0 )*(Y)   ,   (Y) = (         0   0.15647         0 )*(YO)           are defined as:
(ZO)   (         0         0   7.84800 ) (Z)   ,   (Z)   (         0         0   0.12742 ) (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 I4/mcm                No: 140, Laue:4/mmm [Hall: -I 4 2c          ]

Lattice Type tI,  Centric,   Tetragonal, Order  32( 8) [Schoenflies: D4h^18    ]

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

   1              X ,              Y ,              Z
   2            - Y ,              X ,              Z
   3            - X ,            - Y ,              Z
   4              Y ,            - X ,              Z
   5              X ,            - Y ,        1/2 - Z
   6              Y ,              X ,        1/2 - Z
   7            - X ,              Y ,        1/2 - Z
   8            - Y ,            - X ,        1/2 - Z
   9            - X ,            - Y ,            - Z
  10              Y ,            - X ,            - Z
  11              X ,              Y ,            - Z
```

12	- Y ,	X ,	- Z
13	- X ,	Y ,	1/2 + Z
14	- Y ,	- X ,	1/2 + Z
15	X ,	- Y ,	1/2 + Z

16	Y ,	X ,	1/2 + Z
17	1/2 + X ,	1/2 + Y ,	1/2 + Z
18	1/2 - Y ,	1/2 + X ,	1/2 + Z
19	1/2 - X ,	1/2 - Y ,	1/2 + Z
20	1/2 + Y ,	1/2 - X ,	1/2 + Z
21	1/2 + X ,	1/2 - Y ,	- Z
22	1/2 + Y ,	1/2 + X ,	- Z
23	1/2 - X ,	1/2 + Y ,	- Z
24	1/2 - Y ,	1/2 - X ,	- Z
25	1/2 - X ,	1/2 - Y ,	1/2 - Z
26	1/2 + Y ,	1/2 - X ,	1/2 - Z
27	1/2 + X ,	1/2 + Y ,	1/2 - Z
28	1/2 - Y ,	1/2 + X ,	1/2 - Z
29	1/2 - X ,	1/2 + Y ,	Z
30	1/2 - Y ,	1/2 - X ,	Z
31	1/2 + X ,	1/2 - Y ,	Z
32	1/2 + Y ,	1/2 + X ,	Z

```
==================================================================================
Structure Tidy: Standardisation of Inorganic Crystal Structure Data
==================================================================================
References: E.Parthe & L.M.Gelato (1984). Acta Cryst., A40, 169-183.
            L.M.Gelato & E.Parthe (1987). J. Appl. Cryst. 20, 139-143.
            S-Z.Hu & E.Parthe (2004). Chinese J. Struct. Chem. 23 1150-1160.

Input for :  EUSE
Space group symbol : I 4/M C M

Cell parameters :   6.39100  6.39100  7.84800  90.000  90.000  90.000

Number in International Tables : 140

Eu    1  0.00000   0.00000   0.25000
Special position :     0 0 1/4     multiplicity   4  Wyckoff letter: a
All possible special positions for this atom :
    0 0 1/4

Se    1  0.36740   0.13260   0.00000
Special position : x 1/2+x 0       multiplicity   8  Wyckoff letter: h
All possible special positions for this atom :
x 1/2+x 0


x,y,z
-----------------


origin shift  1       0.00000  0.00000  0.00000


Atom Eu    1
Exclude :  2   0.00000   0.00000   0.75000
Exclude :  3   0.50000   0.50000   0.75000
Exclude :  4   0.50000   0.50000   0.25000

Permitted positions :
                      x        y        z            D
        1         0.00000  0.00000  0.25000       0.2500            4a

Chosen :  1   0.00000   0.00000   0.25000     D= 0.2500           4(a)


Atom Se    1
Exclude :  3   0.13260   0.36740   0.50000
Exclude :  4   0.86740   0.63260   0.50000
Exclude :  5   0.36740   0.86740   0.50000
Exclude :  6   0.63260   0.13260   0.50000
Exclude :  7   0.63260   0.86740   0.00000
```

```
Exclude :  8   0.36740   0.13260   0.00000

Permitted positions :
                      x        y        z             D
```

```
        1         0.13260  0.63260  0.00000       0.6463            8h
        2         0.86740  0.36740  0.00000       0.9420            8h

Chosen :  1   0.13260   0.63260   0.00000     D= 0.6463           8(h)


Chosen positions for setting x,y,z
origin shift  0.00000 0.00000 0.00000
atom          x         y         z       occup
Eu    1   0.00000   0.00000   0.25000                 4a
Se    1   0.13260   0.63260   0.00000                 8h
Standardization parameter gamma =   0.8963


origin shift  2       0.00000  0.00000  0.50000


Atom Eu    1
Exclude :  1   0.00000   0.00000   0.75000
Exclude :  3   0.50000   0.50000   0.25000
Exclude :  4   0.50000   0.50000   0.75000

Permitted positions :
                      x        y        z            D
        2         0.00000  0.00000  0.25000       0.2500            4a

Chosen :  2   0.00000   0.00000   0.25000     D= 0.2500           4(a)


Atom Se    1
Exclude :  1   0.13260   0.63260   0.50000
Exclude :  2   0.86740   0.36740   0.50000
Exclude :  3   0.13260   0.36740   0.00000
Exclude :  4   0.86740   0.63260   0.00000
Exclude :  7   0.63260   0.86740   0.50000
Exclude :  8   0.36740   0.13260   0.50000

Permitted positions :
                      x        y        z            D
        5         0.36740  0.86740  0.00000       0.9420            8h
        6         0.63260  0.13260  0.00000       0.6463            8h

Chosen :  6   0.63260   0.13260   0.00000     D= 0.6463           8(h)


Chosen positions for setting x,y,z
origin shift  0.00000 0.00000 0.50000
atom          x         y         z       occup
Eu    1   0.00000   0.00000   0.25000                 4a
Se    1   0.63260   0.13260   0.00000                 8h
Standardization parameter gamma =   0.8963
```

```
Minimum standardization parameter gamma =   0.8963
```

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==================================================================================================
All Possible Settings :
=======================

Setting x,y,z              Origin  0.00000 0.00000 0.00000   Gamma =   0.8963
Gamma/min(Gamma) = 1.0000
Cell parameters :   6.3910  6.3910  7.8480   90.000   90.000   90.000
Eu    1     0.00000  0.00000  0.25000                 4a
Se    1     0.13260  0.63260  0.00000                 8h

sums :      0.13260  0.63260  0.25000


Setting x,y,z              Origin  0.00000 0.00000 0.50000   Gamma =   0.8963
Gamma/min(Gamma) = 1.0000
Cell parameters :   6.3910  6.3910  7.8480   90.000   90.000   90.000
Eu    1     0.00000  0.00000  0.25000                 4a
Se    1     0.63260  0.13260  0.00000                 8h

sums :      0.63260  0.13260  0.25000
```

```
==========================================================================================================
Results for  EUSE
====================================================


Setting x,y,z              origin   0.00000  0.00000  0.00000   gamma =   0.8963

Volume of unit cell :   320.5506

CG parameter (centre of gravity) :   0.3341

(140) I 4/m c m   - h a                                    tI12
-------------------------------------------------------------------------
DATA    EUSE                                              0.8963  0.3341
CELL          6.3910          7.8480
ATOM     Se        8(h)  0.132600.63260 0                                1
ATOM    Eu         4(a)   0      0      1/4                              1


End of STIDY
```

===========
*** N O T I C E ***
===========

- PLATON Reference : Spek, A.L. (2003), J.Appl.Cryst. 36, 7-13

- Output Values (Esd) may have been set to 99, 999 or 9999 to Avoid Format Overflow

- Derived Parameter SU's (= Esd's) may be Incorrect in Cases where Covariances in the Atom Parameters should have been taken into Account (e.g. Those Involving Atoms That were Refined with Constraints)

- ROUNDING, in particular of the Input Coordinate Data, may give deviating values for derived geometry parameters. However, differences should be within the associated esd-range.

- PLATON is NOT a Finished Program. The Implementation of Additional Options is Planned. Some of the More Advanced Features are Experimental and may Contain Loose Ends.

- The Communication of Glitches Encountered will be Appreciated: E-mail: a.l.spek@chem.uu.nl

- Recent versions of PLATON may be obtained by Anonymous FTP from xraysoft.chem.uu.nl

- More INFO can be found on http://www.cryst.chem.uu.nl/platon/

```
================================================================================================================================
Page - Index
==============================================================================

Page   1 --- GENERAL
Page   3 --- Str-Tidy
Page   6 --- SUMMARY



Summary and Remarks : N = NOTE, W = WARNING, E = ERROR
==============================================================================

W: No Cell estimated standard deviation (CESD) given.
N: No S.U.'s (esd) on observed/calculated parameters.
------------------------------------------------------------------------------
N: Number of Ignored Lines on INPUT .....................................    1
          of which blank in column 1 ....................................    1

==============================================================================

:: Input Data from File st.spf - Data Type SPF

:: NORMAL END of PLATON :     7 Pages on:
:: st.lis (ASCII, 132 Characters Wide)
:: st.lps (PostScript Version of .lis)
```