checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx_exp_1230, shelx_exp_2221

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: shelx_exp_1230

```
Bond precision:    Si- O = 0.0081 A          Wavelength=0.71073

Cell:          a=10.0080(2)       b=8.3622(1)        c=13.2994(2)
               alpha=89.987(1)    beta=109.095(2)    gamma=89.978(1)
Temperature:   293 K
```

	Calculated	Reported
Volume	1051.77(3)	1051.77(3)
Space group	C 1	C_1
Hall group	C 1	?
Moiety formula	Fe2 H2 O28 Si8 Sn2, 4(Ca)	?
Sum formula	Ca4 Fe2 H2 O28 Si8 Sn2	Ca8 H4 Fe4.02 O56 Si16 Sn3.98
Mr	1183.61	2367.01
Dx,g cm-3	3.737	3.737
Z	2	1
Mu (mm-1)	5.273	5.272
F000	1139.6	1140.0
F000'	1142.02	
h,k,lmax	14,11,18	14,11,18
Nref	6112[3056]	5918
Tmin,Tmax	0.848,0.984	0.757,1.000
Tmin'	0.840	

```
Correction method= # Reported T Limits: Tmin=0.757 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.94/0.97        Theta(max)= 29.992
```

R(reflections)= 0.0202(5077)   wR2(reflections)= 0.0408(5918)

S = 0.999   Npar= 276

The following ALERTS were generated. Each ALERT has the format
         test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

🔴 Alert level A

```
SYMMG01_ALERT_1_A          Unrecognised _symmetry_space_group_name_H-M
            International Tables space group number is not in the CIF
          From the CIF: _symmetry_space_group_name_H-M       c_1
          Int. Tables space group number for c_1 is    0
SYMMG02_ALERT_1_A        Supplied _symmetry_space_group_name_H-M not recognised
          From the CIF: _symmetry_equiv_pos_as_xyz
                                        x, y, z
                                        x+1/2, y+1/2, z
          These symops generate the Hall space group symbol    c_1
           which is equivalent to the H-M space group symbol
```

🟡 Alert level C

```
STRVA01_ALERT_4_C          Flack test results are ambiguous.
          From the CIF: _refine_ls_abs_structure_Flack      0.370
          From the CIF: _refine_ls_abs_structure_Flack_su      0.040
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT155_ALERT_4_C The Triclinic Unitcell is NOT Reduced .........    Please Do !
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600          9 Report
```

⚪ Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite          6 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .      0.370 Note
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...          2 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...  Please Check
PLAT111_ALERT_2_G ADDSYM Detects New (Pseudo) Centre of Symmetry .        100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem        c        100 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New  Space Group      C2/c Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records          4 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records         22 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records          1 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records          1 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)        293 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )        10% Note
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O14     .      129.7 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O24     .      128.1 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O34     .      127.3 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O44     .      127.7 Degree
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............          7 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         17 Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       60.0 Degree
```

```
   2 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   4 ALERT level C = Check. Ensure it is not caused by an omission or oversight
```

```
    23 ALERT level G = General information/check it is not something unexpected

     7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
     8 ALERT type 2 Indicator that the structure model may be wrong or deficient
     4 ALERT type 3 Indicator that the structure quality may be low
     8 ALERT type 4 Improvement, methodology, query or suggestion
     2 ALERT type 5 Informative message, check
```

Datablock: shelx_exp_2221

```
Bond precision:   Si- O = 0.0108 A          Wavelength=0.71073

Cell:             a=9.9985(3)         b=8.3446(2)        c=13.2760(4)
                  alpha=89.986(3)     beta=109.122(2)    gamma=90.020(2)
Temperature:      297 K

                  Calculated                 Reported
Volume            1046.55(5)                 1046.55(5)
Space group       C 1                        C_1
Hall group        C 1                        ?
Moiety formula    Fe2 H2 O28 Si8 Sn2, 4(Ca)  ?
                                             Ca8 H4 Fe3.97 O56 Si16
Sum formula       Ca4 Fe2 H2 O28 Si8 Sn2     Sn4.03
Mr                1184.68                    2370.16
Dx,g cm-3         3.759                      3.761
Z                 2                          1
Mu (mm-1)         5.307                      5.311
F000              1140.4                     1141.0
F000'             1142.80
h,k,lmax          13,11,18                   13,11,18
Nref              5556[ 2778]                5510
Tmin,Tmax         0.897,0.953                0.749,1.000
Tmin'             0.747

Correction method= # Reported T Limits: Tmin=0.749 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.98/0.99      Theta(max)= 29.000
```

R(reflections)= 0.0356(4747)

wR2(reflections)= 0.0851(5510)

S = 1.050   Npar= 276

The following ALERTS were generated. Each ALERT has the format
        test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

🔴 Alert level A

```
SYMMG01_ALERT_1_A          Unrecognised _symmetry_space_group_name_H-M
              International Tables space group number is not in the CIF
            From the CIF: _symmetry_space_group_name_H-M       c_1
            Int. Tables space group number for c_1 is    0
SYMMG02_ALERT_1_A         Supplied _symmetry_space_group_name_H-M not recognised
            From the CIF: _symmetry_equiv_pos_as_xyz
                                      x, y, z
                                      x+1/2, y+1/2, z
            These symops generate the Hall space group symbol    c_1
             which is equivalent to the H-M space group symbol
```

🟡 Alert level C

```
STRVA01_ALERT_4_C            Flack test results are ambiguous.
            From the CIF: _refine_ls_abs_structure_Flack     0.640
            From the CIF: _refine_ls_abs_structure_Flack_su     0.050
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT155_ALERT_4_C The Triclinic Unitcell is NOT Reduced .........    Please Do !
PLAT907_ALERT_2_C Flack x > 0.5, Structure Needs to be Inverted? .    0.64 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        3 Report
```

⚪ Alert level G

```
FORMU01_ALERT_2_G  There is a discrepancy between the atom counts in the
              _chemical_formula_sum and the formula from the _atom_site* data.
            Atom count from _chemical_formula_sum:H4 Ca8 Fe3.97 O56 Si16 Sn4.03
            Atom count from the _atom_site data:  H4 Ca8 Fe3.984 O56 Si16 Sn4.016
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       6 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension       3 Info
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .    0.640 Note
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       2 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...   Please Check
PLAT111_ALERT_2_G ADDSYM Detects New (Pseudo) Centre of Symmetry .     100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem        c     100 %Fit
PLAT113_ALERT_2_G ADDSYM Suggests Possible Pseudo/New  Space Group   C2/c Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records       4 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records      22 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records       1 Report
PLAT173_ALERT_4_G The CIF-Embedded .res File Contains DANG Records       1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1 )     10% Note
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O14      .   128.2 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O24      .   127.6 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O34      .   127.6 Degree
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O44      .   128.6 Degree
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      7 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).       1 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged   Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..    58.0 Degree
```

```
  2 ALERT level A = Most likely a serious problem – resolve or explain
  0 ALERT level B = A potentially serious problem, consider carefully
  5 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 22 ALERT level G = General information/check it is not something unexpected

  5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 11 ALERT type 2 Indicator that the structure model may be wrong or deficient
  4 ALERT type 3 Indicator that the structure quality may be low
  7 ALERT type 4 Improvement, methodology, query or suggestion
  2 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.
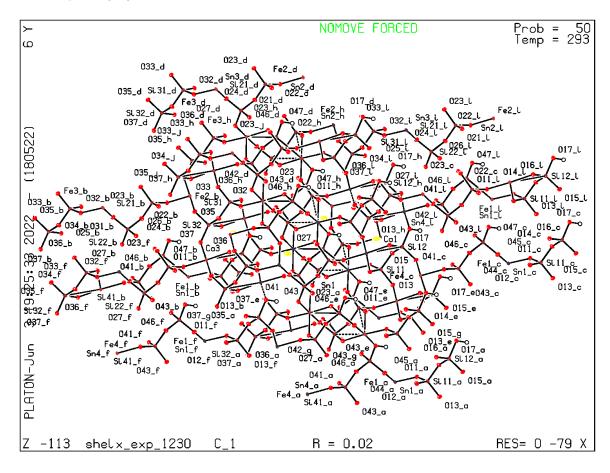
Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_SYMMG01_shelx_exp_1230
;
PROBLEM: Unrecognised _symmetry_space_group_name_H-M
RESPONSE: ...
;
_vrf_SYMMG02_shelx_exp_1230
;
PROBLEM: Supplied _symmetry_space_group_name_H-M not recognised
RESPONSE: ...
```

```
;
_vrf_STRVA01_shelx_exp_1230
;
PROBLEM: Flack test results are ambiguous.
RESPONSE: ...
;
_vrf_PLAT041_shelx_exp_1230
;
PROBLEM: Calc. and Reported SumFormula   Strings  Differ    Please Check
RESPONSE: ...
;
_vrf_PLAT155_shelx_exp_1230
;
PROBLEM: The Triclinic Unitcell is NOT Reduced ..........   Please Do !
RESPONSE: ...
;
_vrf_PLAT911_shelx_exp_1230
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=   0.600         9 Report
RESPONSE: ...
;
_vrf_SYMMG01_shelx_exp_2221
;
PROBLEM: Unrecognised _symmetry_space_group_name_H-M
RESPONSE: ...
;
_vrf_SYMMG02_shelx_exp_2221
;
PROBLEM: Supplied _symmetry_space_group_name_H-M not recognised
RESPONSE: ...
;
_vrf_STRVA01_shelx_exp_2221
;
PROBLEM: Flack test results are ambiguous.
RESPONSE: ...
;
_vrf_PLAT041_shelx_exp_2221
;
PROBLEM: Calc. and Reported SumFormula   Strings  Differ    Please Check
RESPONSE: ...
;
_vrf_PLAT155_shelx_exp_2221
;
PROBLEM: The Triclinic Unitcell is NOT Reduced ..........   Please Do !
RESPONSE: ...
;
_vrf_PLAT907_shelx_exp_2221
;
PROBLEM: Flack x > 0.5, Structure Needs to be Inverted? .      0.64 Check
RESPONSE: ...
;
_vrf_PLAT911_shelx_exp_2221
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=   0.600         3 Report
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 18/05/2022; check.def file version of 17/05/2022

Datablock shelx_exp_1230 - ellipsoid plot