checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: monteneveite

```
Bond precision:  Fe- O = 0.0014 A        Wavelength=0.71073

Cell:            a=12.6093(2)     b=12.6093(2)     c=12.6093(2)
                 alpha=90         beta=90          gamma=90
Temperature:     293 K
```

	Calculated	Reported
Volume	2004.81(10)	2004.80(6)
Space group	I a -3 d	I a -3 d
Hall group	-I 4bd 2c 3	?
Moiety formula	Fe25.09 O96 Sb14.91, 24(Ca)	Fe25.09 O96 Sb14.91, 24(Ca)
Sum formula	Ca24 Fe25.09 O96 Sb14.91	Ca24 Fe25.09 O96 Sb14.91
Mr	5714.77	5714.77
Dx,g cm-3	4.734	4.734
Z	1	1
Mu (mm-1)	10.991	10.991
F000	2660.8	2660.0
F000’	2667.37	
h,k,lmax	21,21,21	20,20,20
Nref	421	401
Tmin,Tmax	0.244,0.489	0.925,0.988
Tmin’	0.133	

```
Correction method= # Reported T Limits: Tmin=0.925 Tmax=0.988
AbsCorr = MULTI-SCAN

Data completeness= 0.952          Theta(max)= 36.530

R(reflections)= 0.0197( 305)      wR2(reflections)= 0.0613( 401)

S = 1.128                Npar= 19
```

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 C

```
PLAT741_ALERT_1_C Bond    Calc 3.15230(10), Rep     3.15230 ......    Missing s.u.
             X        -T              1.555   1.555 ........     #    9 Check
PLAT741_ALERT_1_C Bond    Calc 3.15230(10), Rep     3.15230 ......    Missing s.u.
             X        -T              1.555  50.556 ........     #   10 Check
PLAT741_ALERT_1_C Bond    Calc 3.15230(10), Rep     3.15230 ......    Missing s.u.
             T        -X              1.555  50.656 ........     #   28 Check
```

Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension         1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT017_ALERT_1_G Check Scattering Type Consistency of         Xas         CA
PLAT017_ALERT_1_G Check Scattering Type Consistency of T        as         FE
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large       5.76 Why ?
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...          4 Units
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  )        36% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          4 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2018 Note
```

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

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

Datablock: shelx

```
Bond precision:  Fe- O = 0.0014 A        Wavelength=0.71073

Cell:            a=12.6093(2)     b=12.6093(2)     c=12.6093(2)
                 alpha=90         beta=90          gamma=90
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	Calculated	Reported
Volume	2004.81(10)	2004.80(6)
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Sum formula	Ca24 Fe25.09 O96 Sb14.91	Ca24 Fe25.09 O96 Sb14.91
Mr	5714.77	5714.77
Dx,g cm-3	4.734	4.734
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Mu (mm-1)	10.991	10.991
F000	2660.8	2660.0
F000′	2667.37	
h,k,lmax	21,21,21	20,20,20
Nref	421	401
Tmin,Tmax		
Tmin′	0.133	

Correction method= Not given

Data completeness= 0.952 Theta(max)= 36.530

R(reflections)= 0.0197(305) wR2(reflections)= 0.0613(401)

S = 1.128 Npar= 19

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

SYMM001_ALERT_1_A _symmetry_cell_setting is missing
The cell setting should be one of the following
* triclinic
* monoclinic
* orthorhombic
* tetragonal
* rhombohedral
* trigonal
* hexagonal
* cubic
The following tests will not be performed.
SYMMS_01,SYMMS_02

EXPT005_ALERT_1_A _exptl_crystal_description is missing
Crystal habit description.
The following tests will not be performed.
CRYSR_01

DIFF003_ALERT_1_A _diffrn_measurement_device_type is missing
Diffractometer make and type. Replaces _diffrn_measurement_type.

ATOM002_ALERT_1_A _atom_site_label is missing
Unique label identifying the atom site.

ATOM003_ALERT_1_A _atom_site_fract_x is missing
Fractional coordinates of atom site.

```
ATOM004_ALERT_1_A  _atom_site_fract_y is missing
            Fractional coordinates of atom site.
ATOM005_ALERT_1_A  _atom_site_fract_z is missing
            Fractional coordinates of atom site.
TYPE100_ALERT_1_A  _atom_site_label is not of type char.
TYPE101_ALERT_1_A  _atom_site_fract_x is not of type numb.
TYPE102_ALERT_1_A  _atom_site_fract_y is not of type numb.
TYPE103_ALERT_1_A  _atom_site_fract_z is not of type numb.
GEOM001_ALERT_1_A  _geom_bond_atom_site_label_1 is missing
            Label identifying the atom site 1.
GEOM002_ALERT_1_A  _geom_bond_atom_site_label_2 is missing
            Label identifying the atom site 2.
GEOM003_ALERT_1_A  _geom_bond_distance is missing
            Distance between atom sites 1 and 2.
```

```
  14 ALERT level A = Most likely a serious problem - resolve or explain
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   0 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   0 ALERT level G = General information/check it is not something unexpected

  14 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
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   0 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.

PLATON version of 06/01/2019; check.def file version of 19/12/2018

Datablock monteneveite - ellipsoid plot