checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3116

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: 3116

Bond precision: C-C = 0.0053 A Wavelength=0.71073

Cell: a=12.8025(4) b=18.1923(6) c=17.9925(7)
alpha=90 beta=90.855(3) gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	4190.1(3)	4190.1(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C46 H52 Fe4 N2 O3 Si2	C46 H52 Fe4 N2 O3 Si2
Sum formula	C46 H52 Fe4 N2 O3 Si2	C46 H52 Fe4 N2 O3 Si2
Mr	960.48	960.47
Dx,g cm-3	1.523	1.523
Z	4	4
Mu (mm-1)	1.458	1.458
F000	1992.0	1992.0
F000’	1998.65	
h,k,lmax	16,23,22	16,23,22
Nref	9156	9116
Tmin,Tmax	0.839,0.930	0.870,1.000
Tmin’	0.747	

Correction method= # Reported T Limits: Tmin=0.870 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 27.000

R(reflections)= 0.0431(7194) wR2(reflections)= 0.1035(9116)

S = 1.028 Npar= 526

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

```
PLAT213_ALERT_2_C Atom C6             has ADP max/min Ratio .....       3.7 prolat
PLAT213_ALERT_2_C Atom C10            has ADP max/min Ratio .....       3.7 prolat
PLAT213_ALERT_2_C Atom C40            has ADP max/min Ratio .....       3.2 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1   C   Ueq(max)/Ueq(min) Range      4.5 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1   H Uiso(max)/Uiso(min) Range      4.2 Ratio
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of       C6 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C10 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C39 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of      C40 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      Fe1 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of      Fe4 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......    2.712 Check
```

Alert level G

```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      5.77 Why ?
PLAT793_ALERT_4_G The Model has Chirality at Si1     (Centro SPGR)        R Verify
PLAT793_ALERT_4_G The Model has Chirality at Si2     (Centro SPGR)        R Verify
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min)         4 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       36 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       1 Note
```

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

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  12 ALERT type 2 Indicator that the structure model may be wrong or deficient
   3 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   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 24/11/2016; check.def file version of 23/11/2016

Datablock 3116 - ellipsoid plot