checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3239

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: 3239

Bond precision: C-C = 0.0198 A Wavelength=0.71073

Cell: a=13.7887(10) b=26.7489(19) c=15.0402(18)
alpha=90 beta=101.546(9) gamma=90
Temperature: 173 K

	Calculated	Reported
Volume	5435.1(9)	5435.1(9)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	C16 H26 Fe N Si, Cl	6(C16 H26 Fe N Si), 6(Cl)
Sum formula	C16 H26 Cl Fe N Si	C96 H156 Cl6 Fe6 N6 Si6
Mr	351.77	2110.60
Dx,g cm-3	1.290	1.290
Z	12	2
Mu (mm-1)	1.037	1.037
F000	2232.0	2232.0
F000’	2239.29	
h,k,lmax	17,32,18	17,32,18
Nref	21352[10918]	21323
Tmin,Tmax	0.975,0.990	0.917,1.000
Tmin’	0.901	

Correction method= # Reported T Limits: Tmin=0.917 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.95/1.00 Theta(max)= 26.000

R(reflections)= 0.0765(12047) wR2(reflections)= 0.1450(21323)

S = 1.009 Npar= 1121

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

PLAT213_ALERT_2_A Atom C13 has ADP max/min Ratio ..... 5.4 prolat

Alert level B

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0198 Ang.

Alert level C

PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 9.73 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 2.82 Report
PLAT213_ALERT_2_C Atom C108 has ADP max/min Ratio ..... 3.3 prolat
PLAT213_ALERT_2_C Atom C70 has ADP max/min Ratio ..... 3.2 prolat
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 3.1 Ratio
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) ... 4.4 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C30 -- C71 .. 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N19 -- C69 .. 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C14 -- C47 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N36 -- C166 .. 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C7 -- C134 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C13 -- C62 .. 0.18 Ang.
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C102 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C108 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... Si14 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.1 Note
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H51A .. H84C .. 2.10 Ang.
PLAT413_ALERT_2_C Short Inter XH3 .. XHn H51B .. H82B .. 2.11 Ang.
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Th(Min) ... 10 Report
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 5 Report

Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 1 Report
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 6 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ..... 6.00 Ratio
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage = 17 Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.68) in Resd. # 12 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (0.32) in Resd. # 13 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact Cl2 .. C166 .. 3.18 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl9 .. Cl2 .. 3.19 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 7 Note

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

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
9 ALERT type 4 Improvement, methodology, query or suggestion
1 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*, 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_PLAT213_3239
;
PROBLEM: Atom C13             has ADP max/min Ratio .....        5.4 prolat
RESPONSE: ...
;
# end Validation Reply Form
```

PLATON version of 21/04/2015; check.def file version of 09/03/2015

Datablock 3239 - ellipsoid plot