checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3260_twin1_hklf4

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: 3260_twin1_hklf4

Bond precision: C-C = 0.0071 A Wavelength=0.71073

Cell: a=12.4955(17) b=13.3231(18) c=14.0840(17)
alpha=64.660(12) beta=81.873(11) gamma=69.240(13)
Temperature: 173 K

	Calculated	Reported
Volume	1981.4(5)	1981.4(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C17 H27 Fe N O2 Si), 0.5(C6 H6), H2 O	2(C17 H27 Fe N O2 Si), H2 O, C3 H3
Sum formula	C37 H59 Fe2 N2 O5 Si2	C37 H59 Fe2 N2 O5 Si2
Mr	779.74	779.74
Dx,g cm-3	1.307	1.307
Z	2	2
Mu (mm-1)	0.834	0.834
F000	830.0	830.0
F000’	831.95	
h,k,lmax	15,16,17	15,16,17
Nref	7798	7619
Tmin,Tmax	0.920,0.992	0.858,1.000
Tmin’	0.920	

Correction method= # Reported T Limits: Tmin=0.858 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.977 Theta(max)= 25.999

R(reflections)= 0.0500(2791) wR2(reflections)= 0.0741(7619)

S = 0.657 Npar= 466

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 B

PLAT026_ALERT_3_B Ratio Observed / Unique Reflections too Low .... 37 %

Alert level C

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies
outside the range 0.80 <> 2.00
Goodness of fit given = 0.657

PLAT029_ALERT_3_C	_diffrn_measured_fraction_theta_full Low	0.977	Note
PLAT230_ALERT_2_C	Hirshfeld Test Diff for Si3 -- C29 ..	6.0	su
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C10 -- C40 ..	5.6	su
PLAT331_ALERT_2_C	Small Average Phenyl C-C Dist. C47 -C51_a	1.37	Ang.
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.0071	Ang.
PLAT417_ALERT_2_C	Short Inter D-H..H-D H3 .. H4 ..	2.11	Ang.
PLAT601_ALERT_2_C	Structure Contains Solvent Accessible VOIDS of .	35	Ang3
PLAT906_ALERT_3_C	Large K value in the Analysis of Variance	2.040	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Th(Min) ...	8	Report
PLAT911_ALERT_3_C	Missing # FCF Refl Between THmin & STh/L= 0.600	157	Report

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Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	11	Note
PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3	Report
PLAT180_ALERT_4_G	Check Cell Rounding: # of Values Ending with 0 =	3	
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	6	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	16	Note

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
11 **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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
7 ALERT type 2 Indicator that the structure model may be wrong or deficient
7 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*, 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 21/06/2015; check.def file version of 21/06/2015

Datablock 3260_twin1_hklf4 - ellipsoid plot

