checkCIF/PLATON report

Structure factors have been supplied for datablock(s) mo_b0425_0m

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: mo_b0425_0m

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Bond precision:  C-C = 0.0032 A          Wavelength=0.71073

Cell:          a=9.7419(18)      b=13.252(3)      c=17.228(3)
               alpha=98.993(5)   beta=98.779(5)   gamma=110.464(5)
Temperature:   100 K
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	Calculated	Reported
Volume	2005.9(7)	2005.8(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C36 H60 Fe2 N2 O Si4	C36 H60 Fe2 N2 O Si4
Sum formula	C36 H60 Fe2 N2 O Si4	C36 H60 Fe2 N2 O Si4
Mr	760.92	760.92
Dx,g cm-3	1.260	1.260
Z	2	2
Mu (mm-1)	0.872	0.872
F000	812.0	812.0
F000’	814.19	
h,k,lmax	13,18,24	13,18,23
Nref	11373	11305
Tmin,Tmax	0.774,0.941	0.264,0.308
Tmin’	0.774	

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Correction method= # Reported T Limits: Tmin=0.264 Tmax=0.308
AbsCorr = MULTI-SCAN

Data completeness= 0.994          Theta(max)= 29.678

R(reflections)= 0.0418( 9860)     wR2(reflections)= 0.1206( 11305)

S = 1.132                 Npar= 421
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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

PLAT094_ALERT_2_B Ratio of Maximum / Minimum Residual Density .... 4.12 Report
PLAT919_ALERT_3_B Reflection # Likely Affected by the Beamstop ... 2 Check
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers .... 3 Check
PLAT939_ALERT_3_B Large Value of Not (SHELXL) Weight Optimized S . 450.30 Check

Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 2.20 eA-3
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 2.341 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 4 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 2 Check
PLAT971_ALERT_2_C Check Calcd Residual Density 1.17A From C14 2.18 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 0.72A From Fe2 2.08 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H6 -0.33 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H7 -0.40 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H17A -0.35 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H25 -0.31 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H26 -0.32 eA-3

Alert level G

PLAT154_ALERT_1_G The s.u.’s on the Cell Angles are Equal ..(Note) 0.005 Degree
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min) 3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 60 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Note

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

2 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
8 ALERT type 3 Indicator that the structure quality may be low
1 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 26/02/2017; check.def file version of 21/02/2017

Datablock mo_b0425_0m - ellipsoid plot