checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 3094

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: 3094

Bond precision: C-C = 0.0059 A Wavelength=0.71073

Cell: a=12.3951(4) b=12.5719(4) c=13.6964(5)
alpha=78.754(3) beta=85.109(3) gamma=77.113(3)
Temperature: 150 K

	Calculated	Reported
Volume	2038.65(12)	2038.65(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C40 H50 Fe2 N2 O3 Si2, 2(Cl), H2 O	C40 H50 Fe2 N2 O3 Si2, 2(Cl), H2 O
Sum formula	C40 H52 Cl2 Fe2 N2 O4 Si2	C40 H52 Cl2 Fe2 N2 O4 Si2
Mr	863.62	863.61
Dx,g cm-3	1.407	1.407
Z	2	2
Mu (mm-1)	0.944	0.944
F000	904.0	904.0
F000’	906.55	
h,k,lmax	15,15,16	15,15,16
Nref	8025	8022
Tmin,Tmax	0.797,0.910	0.978,1.000
Tmin’	0.753	

Correction method= # Reported T Limits: Tmin=0.978 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.999

R(reflections)= 0.0517(6707) wR2(reflections)= 0.1337(8022)

S = 1.045 Npar= 492

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

PLAT416_ALERT_2_B Short Intra D-H..H-D H1 .. H3 .. 1.70 Ang.
PLAT420_ALERT_2_B D-H Without Acceptor O4 -- H4B ... Please Check
PLAT936_ALERT_2_B The Embedded .res File Includes a DAMP Command . 50.0 Report

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Alert level C

PLAT213_ALERT_2_C Atom C39 has ADP max/min Ratio ..... 3.4 prolat
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 4.4 Ratio
PLAT222_ALERT_3_C Non-Solvent Resd 1 H Uiso(max)/Uiso(min) Range 4.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C39 -- C40 .. 6.4 s.u.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C38 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C39 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ..... 3.260 Check
PLAT975_ALERT_2_C Check Calcd Residual Density 0.89A From O3 0.40 eA-3
PLAT976_ALERT_2_C Check Calcd Residual Density 0.42A From O4 -0.65 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Note

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 8 Note
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 ..... 2 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT396_ALERT_2_G Deviating Si-O-Si Angle from 150 Deg for O1 138.8 Degree
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
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 10 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min) 4 Note

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
14 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
4 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* 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 3094 - ellipsoid plot

