

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 2925

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: 2925

Bond precision:	C-C = 0.0042 Å	Wavelength=0.71073
Cell:	a=10.3208(4)	b=10.0402(6) c=26.4327(13)
	alpha=90	beta=95.095(4) gamma=90
Temperature:	173 K	
	Calculated	Reported
Volume	2728.2(2)	2728.2(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C28 H38 Fe2 N2 O2 Si	C28 H38 Fe2 N2 O2 Si
Sum formula	C28 H38 Fe2 N2 O2 Si	C28 H38 Fe2 N2 O2 Si
Mr	574.39	574.39
Dx,g cm-3	1.398	1.398
Z	4	4
Mu (mm-1)	1.135	1.135
F000	1208.0	1208.0
F000'	1211.39	
h,k,lmax	13,12,33	13,12,33
Nref	5958	5949
Tmin,Tmax	0.826,0.924	0.935,1.000
Tmin'	0.680	

Correction method= # Reported T Limits: Tmin=0.935 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 26.999

R(reflections)= 0.0398(4459) wR2(reflections)= 0.0903(5949)

S = 1.025 Npar= 322

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

PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C24	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C25	Check



Alert level G

PLAT395_ALERT_2_G	Deviating	X-O-Y	Angle from 120 Deg for	O1	127.2	Degree
PLAT395_ALERT_2_G	Deviating	X-O-Y	Angle from 120 Deg for	O2	124.3	Degree
PLAT910_ALERT_3_G	Missing #	of FCF	Reflection(s) Below	Theta(Min)	2	Note
PLAT912_ALERT_4_G	Missing #	of FCF	Reflections Above	STh/L=	0.600	7 Note
PLAT978_ALERT_2_G	Number	C-C Bonds	with Positive	Residual Density.	1	Note

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- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **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

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 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
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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.

