

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cxy3045

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: cxy3045

Bond precision: C-C = 0.0061 Å Wavelength=1.54178

Cell: a=10.5746(7) b=15.7664(9) c=20.3486(12)
 alpha=90 beta=90 gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	3392.6(4)	3392.6(4)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C44 H35 Fe N O Si	C44 H35 Fe N O Si
Sum formula	C44 H35 Fe N O Si	C44 H35 Fe N O Si
Mr	677.67	677.67
Dx, g cm ⁻³	1.327	1.327
Z	4	4
Mu (mm ⁻¹)	4.177	4.177
F000	1416.0	1416.0
F000'	1415.86	
h, k, lmax	12, 19, 24	12, 18, 24
Nref	6227[3500]	6213
Tmin, Tmax	0.290, 0.274	0.438, 0.753
Tmin'	0.185	

Correction method= # Reported T Limits: Tmin=0.438 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 1.78/1.00 Theta(max)= 68.437

R(reflections)= 0.0373(5457) wR2(reflections)= 0.0914(6213)

S = 0.979 Npar= 436

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

PLAT220_ALERT_2_C	NonSolvent	Resd 1	C	Ueq(max)/Ueq(min)	Range	3.6	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test	Diff for	C4	--C5	.	5.7	s.u.
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of			C1	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of			C2	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of			C5	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of			Fe1	Check
PLAT341_ALERT_3_C	Low	Bond Precision on	C-C Bonds			0.00613	Ang.

● Alert level G

PLAT033_ALERT_4_G	Flack x Value Deviates > 3.0 * sigma from Zero	.	0.034	Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (II)	.	2.24	Info
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed	..	!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	1	Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
3 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.

Datablock cxy3045 - ellipsoid plot

