

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) js_0169_0m_a_sq

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: js_0169_0m_a_sq

Bond precision:	C-C = 0.0062 A	Wavelength=0.71073	
Cell:	a=13.6367(12)	b=8.7801(8)	c=27.099(3)
	alpha=90	beta=96.285(2)	gamma=90
Temperature:	473 K		
	Calculated	Reported	
Volume	3225.1(5)	3225.2(5)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C28 H26 Fe N8, F6 P [+ solvent]	(C28 H26 N8 Fe), (P F6)	
Sum formula	C28 H26 F6 Fe N8 P [+ solvent]	C28 H26 F6 Fe N8 P	
Mr	675.39	675.40	
Dx, g cm ⁻³	1.391	1.391	
Z	4	4	
Mu (mm ⁻¹)	0.583	0.583	
F000	1380.0	1380.0	
F000'	1382.45		
h,k,lmax	17,11,33	17,11,33	
Nref	6648	6622	
Tmin,Tmax	0.783,0.864	0.676,0.745	
Tmin'	0.783		

Correction method= # Reported T Limits: Tmin=0.676 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 26.462

R(reflections)= 0.0571(4696) wR2(reflections)= 0.1683(6622)

S = 1.031 Npar= 416

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

PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00625	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.112	Check
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0	Info

Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	1 Report
PLAT244_ALERT_4_G	Low Solvent Ueq as Compared to Neighbors of	P1 Check
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	57% Note
PLAT432_ALERT_2_G	Short Inter X...Y Contact F143 ..C112	2.94 Ang.
	x,y,z =	1_555 Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	123 A**3
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (III)	2.80 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	11 Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	! Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	26 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1 Note

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
6 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 22/12/2019; check.def file version of 13/12/2019

