

## checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Al13Fe3

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: Al13Fe3**

Bond precision:	Fe-Al = 0.0013 A	Wavelength=0.71073		
Cell:	a=14.5956(9)	b=14.5956(9)	c=7.6929(4)	
	alpha=90	beta=90	gamma=120	
Temperature:	300 K			

	Calculated	Reported
Volume	1419.27 (19)	1419.27 (19)
Space group	R -3 c	R -3 c :H
Hall group	-R 3 2" c	-R 3 2" c
Moiety formula	Al13 Fe3	?
Sum formula	Al13 Fe3	Al78 Fe18
Mr	518.29	3109.74
Dx, g cm-3	3.638	3.638
Z	6	1
Mu (mm-1)	5.685	5.685
F000	1482.0	1482.0
F000'	1492.72	
h, k, lmax	18, 18, 9	18, 18, 9
Nref	367	367
Tmin, Tmax	0.671, 0.711	0.655, 0.746
Tmin'	0.561	

```
Correction method= # Reported T Limits: Tmin=0.655 Tmax=0.746
AbsCorr = MULTI-SCAN
```

Data completeness= 1.000                      Theta (max)= 27.503

```
R(reflections)= 0.0327( 341)      wR2(reflections)=
S = 1.326                        0.0710( 367)
Npar= 28
```

---

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

CRYSC01\_ALERT\_1\_C The word below has not been recognised as a standard identifier.

gray

CRYSC01\_ALERT\_1\_C No recognised colour has been given for crystal colour.

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 3.231 Check

---



### Alert level G

PLAT004\_ALERT\_5\_G Polymeric Structure Found with Maximum Dimension 1 Info  
PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by a Factor ... 6 Check  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 27.43 Why ?  
PLAT883\_ALERT\_1\_G No Info/Value for \_atom\_sites\_solution\_primary . Please Do !  
PLAT969\_ALERT\_5\_G The 'Henn et al.' R-Factor-gap value ..... 4.63 Note  
Predicted wR2: Based on SigI\*\*2 1.53 or SHELX Weight 5.58

---

- 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  
5 **ALERT level G** = General information/check it is not something unexpected
- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
1 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  
0 ALERT type 4 Improvement, methodology, query or suggestion  
2 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.

