

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

Bond precision: C-C = 0.0030 A Wavelength=0.71075

Cell: a=11.4695(8) b=5.8774(4) c=13.609(1)
 alpha=90 beta=91.553(6) gamma=90

Temperature: 173 K

	Calculated	Reported
Volume	917.06(11)	917.06(11)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	F5 Fe, 0.5(C4 H12 N2), C2 H6 N, H2 O	?
Sum formula	C4 H14 F5 Fe N2 O	C4 H14 F5 Fe N2 O
Mr	257.02	257.02
Dx,g cm-3	1.862	1.862
Z	4	4
Mu (mm-1)	1.690	1.690
F000	524.0	524.0
F000'	525.77	
h,k,lmax	13,6,16	13,6,16
Nref	1609	1588
Tmin,Tmax	0.800,0.845	0.711,1.000
Tmin'	0.613	

Correction method= # Reported T Limits: Tmin=0.711 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.987 Theta(max)= 24.999

R(reflections)= 0.0250(1454) wR2(reflections)= 0.0769(1588)

S = 1.045 Npar= 118

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

PLAT355_ALERT_3_C	Long O-H (X0.82,N0.98A) O1S - H1Q .	1.06 Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.595	18 Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF	8 Note
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.63A From O1S	-0.54 eA-3



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	1 Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	6 Report
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1 (III) .	3.03 Info
PLAT909_ALERT_3_G	Percentage of I>2sig(I) Data at Theta(Max) Still	81% Note
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.6 Low
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged	Please Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2 Info

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

0 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
6 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

