

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) A113Fe4_a

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: Al13Fe4 a

Bond precision:	Al-Al = 0.0085 A	Wavelength=0.71073	
Cell:	a=15.498 (4)	b=8.0814 (17)	c=12.488 (3)
	alpha=90	beta=107.790 (8)	gamma=90
Temperature:	300 K		

	Calculated	Reported
Volume	1489.3(6)	1489.2(6)
Space group	C 2/m	C 2/m
Hall group	-C 2y	-C 2y
Moiety formula	Al39 Fe12	?
Sum formula	Al39 Fe12	Al3.25 Fe
Mr	1722.42	143.53
Dx, g cm ⁻³	3.841	3.841
Z	2	24
Mu (mm ⁻¹)	6.823	6.824
F000	1638.0	1638.0
F000'	1650.80	
h, k, lmax	20, 10, 16	18, 9, 16
Nref	1847	1423
Tmin, Tmax	0.618, 0.664	0.552, 0.746
Tmin'	0.500	

Correction method= # Reported T Limits: Tmin=0.552 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.770 Theta (max)= 27.536

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R(reflections)= 0.0803( 756)          wR2(reflections)=
S = 1.064                               0.2230( 1423)
Npar= 128
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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 A

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.820 Why?

Author Response: The high angle diffraction data are not very good.

Alert level B

PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 260 Report

0	8	0,	1	9	0,	3	9	0,	8	4	0,	9	3	0,	10	0	0,
10	2	0,	10	4	0,	11	1	0,	11	3	0,	12	0	0,	12	2	0,
12	4	0,	13	1	0,	13	3	0,	14	0	0,	14	2	0,	14	4	0,
15	1	0,	15	3	0,	16	0	0,	16	2	0,	16	4	0,	17	1	0,
-18	0	1,	-17	1	1,	-17	3	1,	-16	0	1,	-16	2	1,	-16	4	1,
-15	1	1,	-15	3	1,	-15	5	1,	-14	0	1,	-14	2	1,	-14	4	1,
-13	1	1,	-13	3	1,	-12	0	1,	-12	2	1,	-12	4	1,	-11	1	1,
-11	3	1,	-10	2	1,	-10	4	1,	-10	8	1,	-9	3	1,	-5	9	1,
-3	9	1,	-2	8	1,	-1	7	1,	-1	9	1,	0	8	1,	1	9	1,
9	3	1,	10	0	1,	10	2	1,	11	1	1,	11	3	1,	12	0	1,
12	2	1,	13	1	1,	13	3	1,	14	0	1,	14	2	1,	15	1	1,
15	3	1,	16	0	1,	16	2	1,	17	1	1,	-18	0	2,	-17	1	2,
-17	3	2,	-16	0	2,	-16	2	2,	-16	4	2,	-15	1	2,	-15	3	2,
-15	5	2,	-14	0	2,	-14	2	2,	-14	4	2,	-14	6	2,	-13	1	2,
-13	3	2,	-12	0	2,	-12	2	2,	-12	4	2,	-11	1	2,	-11	3	2,
-10	2	2,	-9	3	2,	-7	5	2,	-5	9	2,	-3	9	2,	-2	6	2,

Author Response: The missing FCF Refl(ections) Between Thmin & STh/L = 0.600 260 are caused by the poor high angle diffraction data, actually it has been checked manually that the above listed 260 reflection are too weak to be integrated and included in the solving and refining the structural model.

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.

DIFMN02_ALERT_2_C The minimum difference density is < -0.1*ZMAX*0.75

_refine_diff_density_min given = -2.043

Test value = -1.950

DIFMN03_ALERT_1_C The minimum difference density is < -0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT098_ALERT_2_C Large Reported Min. (Negative) Residual Density -2.04 eA-3

PLAT213_ALERT_2_C Atom Fe2 has ADP max/min Ratio 3.4 prolat

PLAT213_ALERT_2_C Atom Al15 has ADP max/min Ratio 4.0 prolat

PLAT250_ALERT_2_C Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 1) 3.0 Note

PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	8.892	Check
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.24Ang From Al6	2.05	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.87Ang From Al12	1.75	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 1.20Ang From Al1	1.72	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens. 0.47Ang From Al6	1.53	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 1.20Ang From Fe4	-2.19	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.90Ang From Al3	-2.00	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.60Ang From Al2	-1.91	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.71Ang From Fe4	-1.84	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 1.39Ang From Al8	-1.77	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.81Ang From Al4	-1.67	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 1.14Ang From Al3	-1.64	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.54Ang From Al6	-1.59	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 0.99Ang From Fe1	-1.59	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 1.43Ang From Al2	-1.55	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens. 1.68Ang From Al13	-1.53	eA-3
PLAT973_ALERT_2_C	Check Calcd Positive Resid. Density on Fe2	1.35	eA-3

● Alert level G

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	20	Report
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3	Info
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.083	Check
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT177_ALERT_4_G	The CIF-Embedded .res File Contains DELU Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	104	Note
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please	Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min). 0 0 1,	1	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	119	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	2.8	Low
PLAT950_ALERT_5_G	Calculated (ThMax) and CIF-Reported Hmax Differ	2	Units
PLAT956_ALERT_1_G	Calculated (ThMax) and Actual (FCF) Hmax Differ	2	Units
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	1.66	Note

Predicted wR2: Based on SigI**2 13.43 or SHELX Weight 21.96

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

- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 22 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
 4 ALERT type 4 Improvement, methodology, query or suggestion
 3 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.

