

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20221017_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: 20221017_a

Bond precision: Al-Al = 0.0040 Å Wavelength=0.71073

Cell: a=4.8569(5) b=6.4389(7) c=8.7323(10)
 alpha=87.837(4) beta=74.463(4) gamma=83.060(4)
Temperature: 300 K

	Calculated	Reported
Volume	261.18(5)	261.18(5)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	Al _{12.48} Fe _{6.52}	?
Sum formula	Al _{12.48} Fe _{6.52}	Al _{13.12} Fe _{1.63}
Mr	700.74	175.19
Dx, g cm ⁻³	4.455	4.455
Z	1	4
Mu (mm ⁻¹)	9.802	9.803
F000	331.7	332.0
F000'	334.69	
h,k,lmax	6,8,11	6,8,11
Nref	1212	1210
Tmin,Tmax	0.499,0.745	0.533,0.746
Tmin'	0.452	

Correction method= # Reported T Limits: Tmin=0.533 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.998 Theta(max)= 27.571

R(reflections)= 0.0543(907)	wR2(reflections)=
S = 1.057	0.1044(1210)
Npar= 89	

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

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

CRYSC01_ALERT_1_C The word below has not been recognised as a standard
identifier.
drak

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.

PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 6.914 Check

PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.63Ang From Al2 1.59 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.250 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 5.68 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.004 Degree
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1) 10% Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 2 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value 1.68 Note
Predicted wr2: Based on SigI**2 6.21 or SHELX Weight 10.26

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **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

- 7 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
2 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

