

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) exp_299

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: exp_299

Bond precision: C-C = 0.0052 A Wavelength=0.71073

Cell: a=15.4883(9) b=13.6013(7) c=16.6081(10)
 alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	3498.7(3)	3498.7(3)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C15 H21 Fe O6	C15 H21 Fe O6
Sum formula	C15 H21 Fe O6	C15 H21 Fe O6
Mr	353.17	353.17
Dx,g cm-3	1.341	1.341
Z	8	8
Mu (mm-1)	0.885	0.885
F000	1480.0	1480.0
F000'	1483.48	
h,k,lmax	19,17,21	19,17,21
Nref	3850	3851
Tmin,Tmax	0.844,0.893	0.845,0.910
Tmin'	0.821	

Correction method= # Reported T Limits: Tmin=0.845 Tmax=0.910
AbsCorr = ANALYTICAL

Data completeness= 1.000 Theta(max)= 27.103

R(reflections)= 0.0519(2065) wR2(reflections)= 0.1251(3851)

S = 1.010 Npar= 205

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**

RINTA01_ALERT_3_C The value of Rint is greater than 0.12
Rint given 0.137

PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C8	Check
PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C13	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C2	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C4	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C7	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C9	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C12	Check
PLAT242_ALERT_2_C	Low	'MainMol'	Ueq as Compared to Neighbors of	C14	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		20.328	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance		4.473	Check

● **Alert level G**

PLAT012_ALERT_1_G	No	_shelx_res_checksum	Found in CIF	Please	Check
PLAT020_ALERT_3_G	The Value of Rint is Greater Than 0.12		0.137	Report	
PLAT199_ALERT_1_G	Reported	_cell_measurement_temperature (K)	293	Check	
PLAT200_ALERT_1_G	Reported	_diffrn_ambient_temperature (K)	293	Check	
PLAT794_ALERT_5_G	Tentative Bond Valency for Fe1	(III)	.	3.20	Info	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.			0	Info	

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
11 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected
- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
0 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

PLATON version of 05/12/2020; check.def file version of 05/12/2020

