

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 0785_cg_0m

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: 0785_cg_0m

Bond precision: C-C = 0.0031 A Wavelength=0.71073

Cell: a=12.148(2) b=11.104(2) c=19.365(4)
 alpha=90 beta=101.252(8) gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	2562.0(8)	2562.0(8)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C50 H78 Fe2 O4 P2	C50 H78 Fe2 O4 P2
Sum formula	C50 H78 Fe2 O4 P2	C50 H78 Fe2 O4 P2
Mr	916.76	916.76
Dx,g cm-3	1.188	1.188
Z	2	2
Mu (mm-1)	0.668	0.668
F000	984.0	984.0
F000'	986.08	
h,k,lmax	16,15,26	16,14,26
Nref	6673	6842
Tmin,Tmax	0.787,0.853	0.649,0.745
Tmin'	0.787	

Correction method= # Reported T Limits: Tmin=0.649 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.025 Theta(max)= 28.797

R(reflections)= 0.0422(6093) wR2(reflections)= 0.1031(6842)

S = 1.042 Npar= 375

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**

PLAT329_ALERT_4_C	Carbon Atom Hybridisation Unclear for	C15B	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.137	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	23	Report
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF	14	Note

● **Alert level G**

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	13	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	13	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	15	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Fe1 --P1	8.0	s.u.
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	38%	Note
PLAT412_ALERT_2_G	Short Intra XH3 .. XHn H2C ..H17B .	1.95	Ang.
	x,y,z =	1_555	Check
PLAT773_ALERT_2_G	Check long C-C Bond in CIF: C15B --C22	1.77	Ang.
PLAT793_ALERT_4_G	Model has Chirality at C4 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C15A (Centro SPGR)	S	Verify
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	96	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	4	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	54	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	6	Note

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
17 **ALERT level G** = General information/check it is not something unexpected

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

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