

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) deh148

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: deh148

Bond precision:	C-C = 0.0043 A	Wavelength=0.71073
Cell:	a=13.8409(9)	b=22.4674(15) c=21.2115(14)
	alpha=90	beta=106.780(4) gamma=90
Temperature:	150 K	
	Calculated	Reported
Volume	6315.3(7)	6315.3(7)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C69 H51 Fe N9, 2(F6 P), C H2 Cl2	C69 H51 Fe N9, C H2 Cl2, 2(F6 P)
Sum formula	C70 H53 Cl2 F12 Fe N9 P2	C70 H53 Cl2 F12 Fe N9 P2
Mr	1436.91	1436.90
Dx,g cm-3	1.511	1.511
Z	4	4
Mu (mm-1)	0.462	0.462
F000	2936.0	2936.0
F000'	2940.86	
h,k,lmax	18,29,27	18,29,27
Nref	14594	14536
Tmin,Tmax	0.957,0.968	0.677,0.746
Tmin'	0.955	

Correction method= # Reported T Limits: Tmin=0.677 Tmax=0.746

AbsCorr = MULTI-SCAN

Data completeness= 0.996 Theta(max)= 27.555

R(reflections)= 0.0560(9373) wR2(reflections)= 0.1215(14536)

S = 1.019 Npar= 868

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

PLAT410_ALERT_2_C	Short Intra H...H Contact	H3	..H15	.	1.96	Ang.
			x,y,z	=	1_555	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance			5.340	Check
PLAT910_ALERT_3_C	Missing # of FCF Reflection(s) Below Theta(Min).				8	Note
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600			2	Report



Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ				Please	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large			8.82	Why ?
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	Fel	--C14	.	6.5	s.u.
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of				P1	Check
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of				P2	Check
PLAT794_ALERT_5_G	Tentative Bond Valency for Fel	(III)	.		2.98	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600			47	Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...				1	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.				3	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
9 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
3 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.

