

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: naka104

Bond precision:	C-C = 0.0153 A	Wavelength=0.71073
Cell:	a=12.2585(6) b=15.5003(7) c=12.9367(6)	
	alpha=90 beta=110.806(1) gamma=90	
Temperature:	103 K	
	Calculated	Reported
Volume	2297.81(19)	2297.81(19)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	C54 H44 Fe P2 Pt Si, C H2 Cl2	C54 H44 Fe P2 Pt Si, C H2 Cl2
Sum formula	C55 H46 Cl2 Fe P2 Pt Si	C55 H46 Cl2 Fe P2 Pt Si
Mr	1118.78	1118.79
Dx, g cm ⁻³	1.617	1.617
Z	2	2
Mu (mm ⁻¹)	3.607	3.607
F000	1116.0	1116.0
F000'	1114.78	
h,k,lmax	14,18,15	14,18,15
Nref	8569[4455]	8350
Tmin,Tmax	0.528,0.835	0.504,0.840
Tmin'	0.448	

Correction method= # Reported T Limits: Tmin=0.504 Tmax=0.840
AbsCorr = EMPIRICAL

Data completeness= 1.87/0.97 Theta(max)= 25.500

R(reflections)= 0.0484(7924) wR2(reflections)= 0.1191(8350)

S = 1.018 Npar= 571

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

STRVA01_ALERT_4_C Flack test results are ambiguous.
 From the CIF: `_refine_ls_abs_structure_Flack` 0.501
 From the CIF: `_refine_ls_abs_structure_Flack_su` 0.008
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) 7.80 Note
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.62 Report
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.01528 Ang.
PLAT420_ALERT_2_C D-H Without Acceptor Si1 -- H2 ... Please Check
PLAT420_ALERT_2_C D-H Without Acceptor Si1 -- H3 ... Please Check

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero . 0.501 Note
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 14.24 Why ?
PLAT860_ALERT_3_G Number of Least-Squares Restraints 2 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2016 Note

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

0 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.

