

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: shelxl

Bond precision:	C-C = 0.0244 A	Wavelength=0.71073	
Cell:	a=10.8500(7)	b=9.5950(3)	c=19.8390(13)
	alpha=90	beta=105.962(2)	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	1985.72(19)	1985.72(19)	
Space group	P 21/c	P2(1)/c	
Hall group	-P 2ybc	?	
Moiety formula	C40 H36 Au2 Fe N2 P2 S4	?	
Sum formula	C40 H36 Au2 Fe N2 P2 S4	C40 H36 Au2 Fe N2 P2 S4	
Mr	1184.72	1184.67	
Dx,g cm-3	1.981	1.981	
Z	2	2	
Mu (mm-1)	8.053	8.053	
F000	1136.0	1136.0	
F000'	1130.70		
h,k,lmax	14,12,25	14,12,25	
Nref	4520	4473	
Tmin,Tmax	0.154,0.170		
Tmin'	0.116		

Correction method= Not given

Data completeness= 0.990 Theta(max)= 27.400

R(reflections)= 0.0582(2551) wR2(reflections)= 0.1861(4473)

S = 1.049 Npar= 233

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 B

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds 0.0244 Ang.

Alert level C

PLAT057_ALERT_3_C Correction for Absorption Required RT(exp) ... 1.11
PLAT234_ALERT_4_C Large Hirshfeld Difference N1 -- C1 .. 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C2 -- C3 .. 0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C23 -- C24 .. 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C31 -- C32 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C33 -- C34 .. 0.22 Ang.
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for C2 Check
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C2 - C3 ... 1.42 Ang.

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT128_ALERT_4_G Alternate Setting for Input Space-Group P21/c P21/n Note
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 = 3
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected
- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
7 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*, 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 18/09/2013; check.def file version of 12/09/2013

