

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) test3

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: test3

Bond precision:	C-C = 0.0072 Å	Wavelength=0.71073
Cell:	a=9.8320(9) b=14.3623(13) c=13.9396(13)	
	alpha=90 beta=91.5485(14) gamma=90	
Temperature:	90 K	
	Calculated	Reported
Volume	1967.7(3)	1967.7(3)
Space group	P 21/c	P2(1)/c
Hall group	-P 2ybc	?
Moiety formula	C16 H12 Au2 F2 Fe N6	?
Sum formula	C16 H12 Au2 F2 Fe N6	C16 H12 Au2 F2 Fe N6
Mr	776.11	776.10
Dx,g cm-3	2.620	2.620
Z	4	4
Mu (mm-1)	15.633	15.633
F000	1408.0	1408.0
F000'	1395.17	
h,k,lmax	14,21,20	14,20,20
Nref	6486	5866
Tmin,Tmax	0.228,0.286	0.304,0.368
Tmin'	0.192	

Correction method= # Reported T Limits: Tmin=0.304 Tmax=0.368
AbsCorr = EMPIRICAL

Data completeness= 0.904 Theta(max)= 31.350

R(reflections)= 0.0281(4247) wR2(reflections)= 0.0550(5866)

S = 1.011 Npar= 250

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

PLAT780_ALERT_1_B Coordinates do not Form a Properly Connected Set Please Do !

Alert level C

PLAT972_ALERT_2_C Check Calcd Residual Density 0.78A From Aul -1.55 eA-3
PLAT977_ALERT_2_C Check the Negative Difference Density on H1 -0.67 eA-3
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Note

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT005_ALERT_5_G No Embedded Refinement Details found in the CIF Please Do !
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Au2 -- C16 .. 5.5 s.u.
PLAT301_ALERT_3_G Main Residue Disorder(Resd 1).. 4 % Note
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) . 1.13 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 38 Check
F1 -C2 -H2 1.555 1.555 1.555 1.50 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF # 47 Check
F2 -C4 -H4 1.555 1.555 1.555 7.20 Deg.
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2014 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 619 Note

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
1 **ALERT level B** = A potentially serious problem, consider carefully
3 **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
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
2 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.

