

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) test_0

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: test_0

Bond precision: C-C = 0.0158 Å Wavelength=0.71073

Cell: a=21.658(2) b=13.7647(15) c=15.5895(17)
 alpha=90 beta=90 gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	4647.5(8)	4647.4(9)
Space group	P b c n	Pbcn
Hall group	-P 2n 2ab	?
Moiety formula	C16 H8 Au2 Fe N8, C3 N	?
Sum formula	C19 H8 Au2 Fe N9	C19 H8 Au2 Fe N9
Mr	812.13	812.13
Dx,g cm-3	2.321	2.321
Z	8	8
Mu (mm-1)	13.235	13.236
F000	2952.0	2952.0
F000'	2925.97	
h,k,lmax	28,18,20	28,17,20
Nref	5451	5443
Tmin,Tmax	0.016,0.054	0.052,0.159
Tmin'	0.000	

Correction method= # Reported T Limits: Tmin=0.052 Tmax=0.159
AbsCorr = EMPIRICAL

Data completeness= 0.999 Theta(max)= 27.700

R(reflections)= 0.0411(3533) wR2(reflections)= 0.1197(5443)

S = 1.050 Npar= 284

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 A

PLAT430_ALERT_2_A Short Inter D...A Contact N1 ..N10 . 2.57 Ang.
3/2-x,3/2-y,1/2+z = 2_665 Check

Author Response: The guest molecules should be dynamic positional disorder. So, the steric hindrance between N(1), N(6) and guest molecules should be avoided by the rotational motion.

PLAT430_ALERT_2_A Short Inter D...A Contact N6 ..N10 . 2.33 Ang.
3/2-x,3/2-y,1/2+z = 2_665 Check

Author Response: The guest molecules should be dynamic positional disorder. So, the steric hindrance between N(1), N(6) and guest molecules should be avoided by the rotational motion.

Alert level B

PLAT216_ALERT_3_B Disordered C19 (An/Solv) ADP max/min Ratio 7.9 Note
PLAT934_ALERT_3_B Number of (Iobs-Icalc)/SigmaW > 10 Outliers 2 Check

Alert level C

PLAT220_ALERT_2_C Non-Solvent Resd 1 N Ueq(max)/Ueq(min) Range 3.9 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C5 --C6 0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N9 --C22 0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C21 --C22 0.16 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds 0.0158 Ang.
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.82A From N9 2.07 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.04A From N2 1.64 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.70A From C18 1.51 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.09A From C22 -2.08 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.13A From C20 -1.90 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.07A From N10 -1.86 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.24A From N9 -1.80 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 8 Note
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 !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 53.04 Why ?
PLAT300_ALERT_4_G Atom Site Occupancy of N9 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of N10 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C17 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C18 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C19 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C20 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C21 Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 88% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact N10 ..C14 2.83 Ang.
3/2-x,3/2-y,-1/2+z = 2_664 Check

PLAT432_ALERT_2_G Short Inter X...Y Contact	N10 ..C1	2.84 Ang.
	3/2-x,3/2-y,-1/2+z =	2_664 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C1 ..C20	2.97 Ang.
	3/2-x,3/2-y,1/2+z =	2_665 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C10 ..C18	3.16 Ang.
	1-x,y,3/2-z =	3_656 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd)	.	1.21 Ratio
PLAT860_ALERT_3_G Number of Least-Squares Restraints	16 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL		2018 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600	7 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		1 Info

2 **ALERT level A** = Most likely a serious problem - resolve or explain
 2 **ALERT level B** = A potentially serious problem, consider carefully
 12 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 21 **ALERT level G** = General information/check it is not something unexpected

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 17 ALERT type 2 Indicator that the structure model may be wrong or deficient
 4 ALERT type 3 Indicator that the structure quality may be low
 14 ALERT type 4 Improvement, methodology, query or suggestion
 2 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.

