

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) xs0846a

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: xs0846a

Bond precision:	C-C = 0.0118 Å	Wavelength=1.54178
Cell:	a=8.9838(2)	b=20.6008(5) c=19.6703(6)
	alpha=90	beta=102.450(3) gamma=90
Temperature:	110 K	
	Calculated	Reported
Volume	3554.84(16)	3554.84(16)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C36 H28 Au2 Cl2 O P2, 0.279(C H Cl3), 0.721(C3 H6 O)	C36 H28 Au2 Cl2 O P2, 0.279(C H Cl3), 0.721(C3 H6 O)
Sum formula	C38.44 H32.61 Au2 Cl2.84 O1.72 P2	C38.44 H32.61 Au2 Cl2.84 O1.72 P2
Mr	1078.54	1078.64
Dx,g cm-3	2.015	2.015
Z	4	4
Mu (mm-1)	18.371	18.373
F000	2053.0	2053.0
F000'	2028.06	
h,k,lmax	11,25,24	11,25,24
Nref	6967	8199
Tmin,Tmax	0.382,0.576	0.154,0.686
Tmin'	0.026	

Correction method= # Reported T Limits: Tmin=0.154 Tmax=0.686
AbsCorr = ANALYTICAL

Data completeness= 1.177 Theta(max)= 71.898

R(reflections)= 0.0323(7196) wR2(reflections)= 0.0783(8199)

S = 0.992 Npar= 453

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

PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01175 Ang.



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	7	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	8	Report
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	2	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	2	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Au1 --Cl1 .	7.1	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Au2 --Cl2 .	7.3	s.u.
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 2)	100%	Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 3)	100%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 2	1.40	Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 3	7.21	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C23 ..C33	3.17	Ang.
	-1+x,y,z =	1_455	Check
PLAT434_ALERT_2_G	Short Inter HL..HL Contact Cl1 ..Cl4	3.31	Ang.
	x,1/2-y,-1/2+z =	4_565	Check
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels	6	Note
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	57	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	102	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law [1 0 2] Est.d BASF	0.26	Check
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law [1 0 0] Est.d BASF	0.25	Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	2	Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **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
7 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
12 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.

