

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) xs0849a

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: xs0849a

Bond precision: C-C = 0.0149 Å

Wavelength=1.54178

Cell: a=10.9408(3) b=13.9559(4) c=22.9525(8)
 alpha=88.551(3) beta=87.044(3) gamma=89.587(2)
Temperature: 110 K

	Calculated	Reported
Volume	3498.74(19)	3498.74(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C36 H26 Au2 Cl O P2, F6 Sb	C36 H26 Au2 Cl O P2, F6 Sb
Sum formula	C36 H26 Au2 Cl F6 O P2 Sb	C72 H52 Au4 Cl2 F12 O2 P4 Sb2
Mr	1201.66	2403.28
Dx, g cm-3	2.281	2.281
Z	4	2
Mu (mm-1)	23.648	23.648
F000	2240.0	2240.0
F000'	2214.16	
h,k,lmax	13,17,28	13,17,28
Nref	13727	15046
Tmin,Tmax	0.111,0.307	0.142,0.446
Tmin'	0.031	

Correction method= # Reported T Limits: Tmin=0.142 Tmax=0.446

AbsCorr = ANALYTICAL

Data completeness= 1.096

Theta(max)= 71.896

R(reflections)= 0.0382(13204)

wR2(reflections)= 0.1116(15046)

S = 1.038

Npar= 884

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

PLAT241_ALERT_2_C	High	'MainMol'	Ueq as Compared to Neighbors of	C11B	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	Sb1	Check
PLAT244_ALERT_4_C	Low	'Solvent'	Ueq as Compared to Neighbors of	Sb2	Check
PLAT342_ALERT_3_C	Low	Bond Precision on	C-C Bonds	0.01491	Ang.
PLAT911_ALERT_3_C	Missing	FCF Refl Between	Thmin & STh/L=	0.600	16 Report



Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C72 H52 Au4 Cl2 F12 O2 P4 Sb2
Atom count from _chemical_formula_moiety:C36 H26 Au2 Cl1 F6 O1 P2 Sb1

PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	6	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	2.00	Check
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	2	Report
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1A	104.5	Degree
PLAT398_ALERT_2_G	Deviating C-O-C Angle From 120 for O1B	105.7	Degree
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb1 (V)	5.02	Info
PLAT794_ALERT_5_G	Tentative Bond Valency for Sb2 (V)	4.92	Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	57	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	18	Note
PLAT870_ALERT_4_G	ALERTS Related to Twinning Effects Suppressed ..	!	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	28 Note
PLAT931_ALERT_5_G	CIFcalcFCF Twin Law (0 0 1) Est.d BASF	0.34	Check
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	7	Note

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

2 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
6 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

