

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) C__shelx32_PbWCl

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: C__shelx32_PbWCl

Bond precision:	W-Cl = 0.0054 A	Wavelength=0.71073	
Cell:	a=13.4831(10)	b=13.4831(10)	c=9.8247(7)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	1786.1(3)	1786.1(3)	
Space group	P 42/m	P 42/m	
Hall group	-P 4c	-P 4c	
Moiety formula	C126 Pb3 W6	C126 Pb3 W6	
Sum formula	C126 Pb3 W6	C126 Pb3 W6	
Mr	2646.34	2646.37	
Dx,g cm-3	4.921	4.921	
Z	2	2	
Mu (mm-1)	35.264	35.265	
F000	2264.0	2264.0	
F000'	2245.41		
h,k,lmax	16,16,11	16,16,11	
Nref	1682	1680	
Tmin,Tmax	0.919,0.932	0.092,0.604	
Tmin'	0.004		

Correction method= # Reported T Limits: Tmin=0.092 Tmax=0.604
AbsCorr = NUMERICAL

Data completeness= 0.999 Theta(max)= 25.022

R(reflections)= 0.0565(1360) wR2(reflections)= 0.0818(1680)

S = 1.226 Npar= 87

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

PLAT973_ALERT_2_B Check Calcd Positive Residual Density on Pb2 1.77 eA-3

Alert level C

PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C126 Pb3 W6

PLAT906_ALERT_3_C Large K value in the Analysis of Variance 5.428 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.216 Check

PLAT971_ALERT_2_C Check Calcd Residual Density 1.09A From W1 2.09 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.65A From C17 2.05 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.96A From C13 1.94 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 2.04A From C14 1.92 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.92A From C17 1.69 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.02A From Pb2 1.67 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.91A From C18 1.60 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.14A From W2 1.59 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 2.40A From C11 1.54 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density 1.45A From W1 1.51 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.77A From C12 -1.85 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.74A From C18 -1.66 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.58A From C17 -1.63 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 0.65A From Pb2 -1.61 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.77A From C14 -1.58 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 2.24A From C17 -1.58 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.45A From Pb2 -1.55 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.45A From Pb2 -1.55 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.50A From Pb2 -1.55 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 2.25A From C13 -1.52 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.86A From C17 -1.51 eA-3
PLAT972_ALERT_2_C Check Calcd Residual Density 1.59A From Pb2 -1.51 eA-3

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 69.53 Why ?
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature (K) 293 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact C12 .. C18 .. 3.31 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact C17 .. C17 .. 3.23 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact C17 .. C17 .. 3.23 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) 2.44 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2 (II) 2.12 Note
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) Still 76 % Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min) 2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 Note

0 **ALERT level A** = Most likely a serious problem - resolve or explain

1 **ALERT level B** = A potentially serious problem, consider carefully

25 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

12 **ALERT level G** = General information/check it is not something unexpected

2 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data

28 **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

1 **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.

PLATON version of 26/02/2017; check.def file version of 21/02/2017

