

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) PbW6Cl2

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: PbW6Cl2

Bond precision: Pb-Cl = 0.0037 Å Wavelength=0.71073

Cell: a=7.5253(5) b=10.7498(7) c=12.5959(8)
 alpha=111.752(5) beta=98.044(5) gamma=96.224(5)
Temperature: 293 K

	Calculated	Reported
Volume	922.75(11)	922.75(11)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	Cl14 Pb2 W3	Cl14 Pb2 W3
Sum formula	Cl14 Pb2 W3	Cl14 Pb2 W3
Mr	1462.22	1462.23
Dx,g cm-3	5.263	5.263
Z	2	2
Mu (mm-1)	38.817	38.817
F000	1248.0	1248.0
F000'	1236.01	
h,k,lmax	9,12,15	9,12,15
Nref	3367	3164
Tmin,Tmax	0.000,0.021	0.202,0.560
Tmin'	0.000	

Correction method= # Reported T Limits: Tmin=0.202 Tmax=0.560
AbsCorr = NUMERICAL

Data completeness= 0.940 Theta(max)= 25.350

R(reflections)= 0.0320(2594) wR2(reflections)= 0.0638(3164)

S = 1.043 Npar= 173

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

PLAT029_ALERT_3_A _diffn_measured_fraction_theta_full value Low . 0.939 Note

🟡 Alert level B

PLAT911_ALERT_3_B Missing # FCF Refl Between THmin & STh/L= 0.600 199 Report

🟢 Alert level C

PLAT906_ALERT_3_C Large K value in the Analysis of Variance 3.917 Check

PLAT971_ALERT_2_C Check Calcd Residual Density 0.92A From Pb2 1.58 eA-3

⚪ Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.005 Degree
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Pb2 -- Cl7_f .. 9.7 s.u.
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl1 .. Cl13 .. 3.38 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl3 .. Cl3 .. 3.29 Ang.
PLAT434_ALERT_2_G Short Inter HL..HL Contact Cl8 .. Cl8 .. 3.24 Ang.
PLAT794_ALERT_5_G Tentative Bond Valency for Pb1 (II) 2.32 Note
PLAT794_ALERT_5_G Tentative Bond Valency for Pb2 (II) 2.34 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min) 3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 2 Note

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

- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
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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.

