

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw141

Bond precision: C-C = 0.0072 A Wavelength=1.54178

Cell: a=10.8581(2) b=12.5163(2) c=18.3704(3)
 alpha=91.335(2) beta=91.937(2) gamma=102.785(2)

Temperature: 123 K

	Calculated	Reported
Volume	2432.10(7)	2432.10(7)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C24 H21 N2 P Tl2, C24 H21 N2 P, 2(F6 P)	(C24 H21 N2 P)2, Tl2, (F6 P)2
Sum formula	C48 H42 F12 N4 P4 Tl2	C48 H42 F12 N4 P4 Tl2
Mr	1435.50	1435.50
Dx,g cm-3	1.960	1.960
Z	2	2
Mu (mm-1)	14.583	14.583
F000	1376.0	1376.0
F000'	1365.60	
h,k,lmax	12,14,21	12,14,21
Nref	8598	8341
Tmin,Tmax	0.109,0.417	0.002,0.417
Tmin'	0.002	

Correction method= MULTI-SCAN

Data completeness= 0.970 Theta(max)= 66.640

R(reflections)= 0.0362(7663) wR2(reflections)= 0.0963(8341)

S = 1.033 Npar= 631

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

PLAT307_ALERT_2_A Isolated Metal Atom (Unusual !) Tl2

Author Response: The Tl2 ions are part of a coordination polymer and show in the polymeric strands two long coordinative bonds to the neighbouring phosphole ligands accompanied by weak contacts to the PF6- counter ions.

PLAT307_ALERT_2_A Isolated Metal Atom (Unusual !) Tl2_a

Author Response: The Tl2 ions are part of a coordination polymer and show in the polymeric strands two long coordinative bonds to the neighbouring phosphole ligands accompanied by weak contacts to the PF6- counter ions.

PLAT780_ALERT_1_A Coordinates do not Form a Properly Connected Set ?

Author Response: A consequence of the orientation of the repeating units in the unit cell of the polymeric structure.

● **Alert level C**

PLAT029_ALERT_3_C	_diffn_measured_fraction_theta_full	Low	0.97
PLAT083_ALERT_2_C	SHELXL Second Parameter in WGHT	unusually Large.		7.00
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		2.16
PLAT042_ALERT_1_C	Calc. and Rep. MoietyFormula Strings	Differ	?
PLAT066_ALERT_1_C	Predicted and Reported Transmissions	Identical	.	?
PLAT154_ALERT_1_C	The su's on the Cell Angles are Equal	(x 10000)		200 Deg.
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors	for		P3
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors	for		P4

● **Alert level G**

PLAT779_ALERT_4_G	Suspect or Irrelevant (Bond) Angle in CIF		33.80 Deg.
	C9 -N1 -TL2	1.555	1.555	1.555

3 **ALERT level A** = In general: serious problem

0 **ALERT level B** = Potentially serious problem

8 **ALERT level C** = Check and explain

1 **ALERT level G** = General alerts; check

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

4 **ALERT type 2** Indicator that the structure model may be wrong or deficient

1 **ALERT type 3** Indicator that the structure quality may be low

3 **ALERT type 4** Improvement, methodology, query or suggestion

0 **ALERT type 5** Informative message, check

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*, 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 12/11/2008; check.def file version of 12/11/2008

Datablock sw141 - ellipsoid plot

