

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw30c

Bond precision: C-C = 0.0030 A Wavelength=0.71069

Cell: a=11.3378(3) b=17.5125(4) c=18.9823(5)
 alpha=111.9840(11) beta=91.1627(12) gamma=98.9673(10)

Temperature: 120 K

	Calculated	Reported
Volume	3439.48(15)	3439.48(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 Al F36 O4, C24 H21 N2 P T1, C24 H21 N2 P	C16 Al F36 O4, 2 (C24 H21 N2 P), TL
Sum formula	C64 H42 Al F36 N4 O4 P2 T1	C64 H42 Al F36 N4 O4 P2 T1
Mr	1908.32	1908.32
Dx,g cm-3	1.843	1.842
Z	2	2
Mu (mm-1)	2.557	2.557
F000	1868.0	1868.0
F000'	1864.43	
h,k,lmax	14,22,24	14,22,24
Nref	15838	15786
Tmin,Tmax	0.606,0.600	
Tmin'	0.594	

Correction method= Not given

Data completeness= 0.997 Theta(max)= 27.530

R(reflections)= 0.0200(15103) wR2(reflections)= 0.0524(15786)

S = 1.027 Npar= 1121

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

PLAT308_ALERT_2_A Single Bonded Metal Atom (Unusual !) T11

Author Response: The rather long coordinative TI-N, TI-P and TI-Ph bonds are not taken into account by the checkCIF routine.

Alert level B

PLAT431_ALERT_2_B Short Inter HL..A Contact F23 .. F32A .. 2.57 Ang.

Alert level C

PLAT301_ALERT_3_C Main Residue Disorder 10.00 Perc.
PLAT042_ALERT_1_C Calc. and Rep. MoietyFormula Strings Differ ?
PLAT194_ALERT_1_C Missing _cell_measurement_reflns_used datum ?
PLAT234_ALERT_4_C Large Hirshfeld Difference F32B -- C63B .. 0.12 Ang.
PLAT732_ALERT_1_C Angle Calc 128.30(1), Rep 128.30(3) 3.00 su-Ra
P2 -TL1 -P1 1.555 1.555 1.555

Alert level G

PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 12

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- 1 **ALERT level A** = In general: serious problem
1 **ALERT level B** = Potentially serious problem
5 **ALERT level C** = Check and explain
1 **ALERT level G** = General alerts; check
- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check
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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 sw30c - ellipsoid plot

