

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw199V

Bond precision: C-C = 0.0079 A Wavelength=1.54178

Cell: a=18.2485(2) b=18.2485(2) c=30.7963(3)
 alpha=90 beta=90 gamma=120

Temperature: 100 K

	Calculated	Reported
Volume	8881.44(16)	8881.44(16)
Space group	P 61	P 61
Hall group	P 61	P 61
Moiety formula	C16 Al F36 O4, 3(C7 H5 Cr O2 P3), In	C16 Al F36 O4, 3(C7 H5 Cr O2 P3), In
Sum formula	C37 H15 Al Cr3 F36 In O10 P9	C37 H15 Al Cr3 F36 In O10 P9
Mr	1880.02	1880.02
Dx,g cm-3	2.109	2.109
Z	6	6
Mu (mm-1)	11.508	11.508
F000	5460.0	5460.0
F000'	5498.07	
h,k,lmax	22,22,37	22,22,37
Nref	5815[11402]	11252
Tmin,Tmax	0.300,0.345	0.064,0.437
Tmin'	0.001	

Correction method= GAUSSIAN

Data completeness= 1.93/0.99 Theta(max)= 70.820

R(reflections)= 0.0411(11070) wR2(reflections)= 0.1080(11252)

S = 1.030 Npar= 875

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 !) In1

Author Response: There are six coordinative bonds per In⁺ ion. Due to the rather long In-P bond lengths these are not taken into account by the checkCIF routine.

Alert level B

PLAT241_ALERT_2_B	Check High	Ueq as Compared to Neighbors for	07
PLAT241_ALERT_2_B	Check High	Ueq as Compared to Neighbors for	010
PLAT242_ALERT_2_B	Check Low	Ueq as Compared to Neighbors for	All

Alert level C

PLAT213_ALERT_2_C	Atom F5	has ADP max/min Ratio	3.50	prola
PLAT213_ALERT_2_C	Atom F6	has ADP max/min Ratio	3.30	prola
PLAT213_ALERT_2_C	Atom O10	has ADP max/min Ratio	3.30	prola
PLAT220_ALERT_2_C	Large Non-Solvent	F Ueq(max)/Ueq(min) ...	3.71	Ratio
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cr2 -- C8 ..	5.61	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cr3 -- P7 ..	5.27	su
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C22	
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C25	
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C26	
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C27	
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C28	
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C35	
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C37	
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor	2.09	
PLAT143_ALERT_4_C	su on c - Axis Small or Missing (x 100000)	30	Ang.

Alert level G

REFLT03_ALERT_4_G Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the _publ_section_exptl_refinement section of the submitted CIF.

From the CIF: _diffn_reflms_theta_max	70.82
From the CIF: _reflns_number_total	11252
Count of symmetry unique reflns	5815
Completeness (_total/calc)	193.50%
TEST3: Check Friedels for noncentro structure	
Estimate of Friedel pairs measured	5437
Fraction of Friedel pairs measured	0.935
Are heavy atom types Z>Si present	yes

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	12.74
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P1
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P2
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P3
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P4
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P5
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P6
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P7
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P8
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P9

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

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

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

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

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

19 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
11 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 13/08/2009; check.def file version of 12/08/2009

Datablock sw199V - ellipsoid plot

