

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw119

Bond precision: C-C = 0.0076 A Wavelength=1.54178

Cell: a=19.3692(1) b=19.3692(1) c=11.3398(1)
 alpha=90 beta=90 gamma=120

Temperature: 100 K

	Calculated	Reported
Volume	3684.34(4)	3684.34(4)
Space group	P 3 1 c	P 3 1 c
Hall group	P 3 -2c	P 3 -2c
Moiety formula	C16 Al F36 O4, 3(C10 H15 Fe P5), In	C16 Al F36 O4, 3(C10 H15 Fe P5), In
Sum formula	C46 H45 Al F36 Fe3 In O4 P15	C46 H45 Al F36 Fe3 In O4 P15
Mr	2119.72	2119.72
Dx,g cm-3	1.911	1.911
Z	2	2
Mu (mm-1)	11.548	11.548
F000	2084.0	2084.0
F000'	2094.26	
h,k,lmax	23,23,13	22,22,13
Nref	2198[4377]	4118
Tmin,Tmax	0.436,0.500	0.071,0.500
Tmin'	0.001	

Correction method= MULTI-SCAN

Data completeness= 1.87/0.94 Theta(max)= 66.670

R(reflections)= 0.0249(4051) wR2(reflections)= 0.0591(4118)

S = 1.033 Npar= 325

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 !) In

Author Response: There are rather long coordinative bonds between the In ion and the cyclo-P5 rings of the pentaphosphaferrocenes.

Alert level B

PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for 02

Alert level C

PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Fe -- P3 .. 6.74 su
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for A1
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C15
PLAT141_ALERT_4_C su on a - Axis Small or Missing (x 100000) 10 Ang.
PLAT143_ALERT_4_C su on c - Axis Small or Missing (x 100000) 10 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: _diffrn_reflms_theta_max 66.67
From the CIF: _reflms_number_total 4118
Count of symmetry unique reflns 2198
Completeness (_total/calc) 187.35%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 1920
Fraction of Friedel pairs measured 0.874
Are heavy atom types Z>Si present yes
PLAT033_ALERT_4_G Flack x Parameter Value Deviates from Zero -0.01
PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size 0.64 mm
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
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety C8

- 1 **ALERT level A** = In general: serious problem
- 1 **ALERT level B** = Potentially serious problem
- 5 **ALERT level C** = Check and explain
- 9 **ALERT level G** = General alerts; check

- 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 5 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
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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 13/08/2009; check.def file version of 12/08/2009

Datablock sw119 - ellipsoid plot

