

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: SW116V

Bond precision: C-C = 0.0039 A Wavelength=0.71073
Cell: a=18.5884(3) b=20.3265(4) c=20.6636(3)
 alpha=90 beta=90 gamma=90
Temperature: 90 K

	Calculated	Reported
Volume	7807.5(2)	7807.5(2)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C16 Al F36 O4, 2(C6 H4 F2), In	C16 Al F36 O4, 2(C6 H4 F2), In
Sum formula	C28 H8 Al F40 In O4	C28 H8 Al F40 In O4
Mr	1310.14	1310.14
Dx,g cm-3	2.229	2.229
Z	8	8
Mu (mm-1)	0.858	0.858
F000	5040.0	5040.0
F000'	5040.75	
h,k,lmax	25,27,27	25,27,27
Nref	10110	9605
Tmin,Tmax	0.712,0.850	0.677,1.000
Tmin'	0.557	

Correction method= MULTI-SCAN

Data completeness= 0.950 Theta(max)= 28.720

R(reflections)= 0.0357(6202) wR2(reflections)= 0.0838(9603)

S = 0.945 Npar= 667

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 rather long coordinative bonds between the o-difluorobenzene and the In⁺ cation, which are not taken into account by the checkcif routine.

Alert level B

PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full Low 0.95

Alert level C

PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.01

Alert level G

PLAT063_ALERT_4_G Crystal Size Likely too Large for Beam Size 0.67 mm

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

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

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

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

0 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

1 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

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

