

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 | _diffn_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.

