

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw239B

Bond precision: C-C = 0.0095 A

Wavelength=1.54178

Cell: a=11.4693(5) b=12.0694(4) c=14.7956(6)
 alpha=69.285(3) beta=68.390(4) gamma=88.436(3)
Temperature: 123 K

| | Calculated | Reported |
|----------------|--|--|
| Volume | 1768.53(14) | 1768.53(14) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C26 H20 Cu Mo2 N2 O4 P2, C H2 Cl2, B F4 | C26 H20 Cu Mo2 N2 O4 P2, C H2 Cl2, B F4 |
| Sum formula | C27 H22 B Cl2 Cu F4 Mo2 N2 O4 P2 | C27 H22 B Cl2 Cu F4 Mo2 N2 O4 P2 |
| Mr | 913.55 | 913.55 |
| Dx,g cm-3 | 1.715 | 1.715 |
| Z | 2 | 2 |
| Mu (mm-1) | 9.154 | 9.154 |
| F000 | 896.0 | 896.0 |
| F000' | 896.50 | |
| h,k,lmax | 13,14,18 | 13,14,18 |
| Nref | 6701 | 6632 |
| Tmin,Tmax | 0.106,0.178 | 0.074,0.316 |
| Tmin' | 0.009 | |

Correction method= ANALYTICAL

Data completeness= 0.990

Theta(max)= 70.060

R(reflections)= 0.0517(6091)

wR2(reflections)= 0.1512(6632)

S = 1.043

Npar= 406

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 C

| | | | | | | | |
|-------------------|---------------------------|-----------|----------|-----|----|------|----|
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for | C17 | -- | C18 | .. | 5.03 | su |
| PLAT232_ALERT_2_C | Hirshfeld Test Diff (M-X) | Mo2 | -- | C14 | .. | 6.20 | su |
| PLAT232_ALERT_2_C | Hirshfeld Test Diff (M-X) | Cu1 | -- | P1 | .. | 6.24 | su |
| PLAT342_ALERT_3_C | Low Bond Precision on | C-C Bonds | (x 1000) | Ang | .. | 9 | |

| | | | |
|-------------------|---|------|------|
| PLAT431_ALERT_2_C | Short Inter HL..A Contact C11 .. O3 .. | 3.11 | Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C17 -- C20 .. | 0.16 | Ang. |
| PLAT244_ALERT_4_C | Low 'Solvent' Ueq as Compared to Neighbors of | | C1S |
| PLAT244_ALERT_4_C | Low 'Solvent' Ueq as Compared to Neighbors of | | B1 |

● **Alert level G**

| | | | |
|-------------------|--|--------|------|
| PLAT072_ALERT_2_G | SHELXL First Parameter in WGHT Unusually Large.. | 0.10 | |
| PLAT605_ALERT_4_G | Structure Contains Solvent Accessible VOIDS of . | 224.00 | A**3 |
| PLAT720_ALERT_4_G | Number of Unusual/Non-Standard Labels | | 2 |

0 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
8 **ALERT level C** = Check and explain
3 **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
1 ALERT type 3 Indicator that the structure quality may be low
5 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

