checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: swr6

Bond precision: C-C = 0.0096 A Wavelength=0.71073

Cell: **a=13.8598(9)** **b=13.9687(9)** **c=17.3480(12)**
alpha=77.539(4) **beta=76.183(4)** **gamma=76.205(4)**
Temperature: **100 K**

	Calculated	Reported
Volume	3122.1(4)	3122.1(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C42 H37 Cu2 Mo2 N4 O4 P3, 2(B F4)	C42 H37 Cu2 Mo2 N4 O4 P3, 2(B F4)
Sum formula	C42 H37 B2 Cu2 F8 Mo2 N4 O4 P3	C42 H37 B2 Cu2 F8 Mo2 N4 O4 P3
Mr	1247.27	1247.27
Dx,g cm-3	1.327	1.327
Z	2	2
Mu (mm-1)	1.200	1.200
F000	1236.0	1236.0
F000’	1231.51	
h,k,lmax	17,17,21	17,17,21
Nref	12823	12598
Tmin,Tmax	0.656,0.787	0.619,0.787
Tmin’	0.613	

Correction method= MULTI-SCAN

Data completeness= 0.982 **Theta(max)= 26.390**

R(reflections)= 0.0649(9804) **wR2(reflections)= 0.2039(12598)**

S = 1.094 **Npar= 624**

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

DIFMX01_ALERT_2_C The maximum difference density is > 0.1*ZMAX*0.75
_refine_diff_density_max given = 3.405
Test value = 3.150
DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75

The relevant atom site should be identified.

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.68
PLAT097_ALERT_2_C Large Reported Max. (Positive) Residual Density 3.40 eA-3
PLAT213_ALERT_2_C Atom C30 has ADP max/min Ratio ..... 3.20 prola
PLAT213_ALERT_2_C Atom C31 has ADP max/min Ratio ..... 3.30 prola
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.32 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Ueq(max)/Ueq(min) ... 3.22 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C29 -- C30 .. 5.30 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo1 -- C33 .. 7.03 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo2 -- P2 .. 7.69 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo2 -- C38 .. 5.03 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu1 -- P1 .. 6.85 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu2 -- P1 .. 6.55 su
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C30
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C33
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C34
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C36
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Mo1
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for Mo2
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C101
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 10
PLAT432_ALERT_2_C Short Inter X...Y Contact O3 .. C4A .. 2.94 Ang.
PLAT432_ALERT_2_C Short Inter X...Y Contact O4 .. C202 .. 2.98 Ang.
PLAT194_ALERT_1_C Missing _cell_measurement_reflns_used datum .... ?
PLAT234_ALERT_4_C Large Hirshfeld Difference C35 -- C36 .. 0.15 Ang.
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of B1
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of B2

Alert level G

PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large.. 0.13
PLAT301_ALERT_3_G Note: Main Residue Disorder ..... 3.00 Perc.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 36
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal (x 10000) 400 Deg.
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure !
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 16

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0 **ALERT level A** = In general: serious problem
0 **ALERT level B** = Potentially serious problem
28 **ALERT level C** = Check and explain
6 **ALERT level G** = General alerts; check

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
22 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 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

Datablock swr6 - ellipsoid plot