checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: sw251

Bond precision: C-C = 0.0041 A   Wavelength=1.54178

Cell: a=22.8474(4)   b=13.3251(2)   c=19.0375(4)
                 alpha=90   beta=108.928(2)   gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	5482.45(18)	5482.45(18)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C22 H14 Cu Mo2 N2 O4 P2, C2 H3 N, B F4	C22 H14 Cu Mo2 N2 O4 P2, C2 H3 N, B F4
Sum formula	C24 H17 B Cu F4 Mo2 N3 O4 P2	C24 H17 B Cu F4 Mo2 N3 O4 P2
Mr	815.59	815.59
Dx,g cm-3	1.976	1.976
Z	8	8
Mu (mm-1)	9.976	9.976
F000	3184.0	3184.0
F000'	3179.84	
h,k,lmax	27,15,22	26,15,22
Nref	4853	4778
Tmin,Tmax	0.453,0.689	0.412,0.702
Tmin'	0.123	

Correction method= ANALYTICAL

Data completeness= 0.985   Theta(max)= 66.610

R(reflections)= 0.0247(4164)   wR2(reflections)= 0.0665(4778)

S = 1.036   Npar= 373

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**
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo1   -- P1   ..   7.51 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo1   -- C1   ..   6.13 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo1   -- C2   ..   5.30 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo2   -- C3   ..   6.30 su

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PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Mo2    -- C4      ..       8.90 su
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⬤ Alert level G
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PLAT333_ALERT_2_G Check Large Av C6-Ring C-C Dist. C18    -C22          1.43 Ang.
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 0 ALERT level A = In general: serious problem
 0 ALERT level B = Potentially serious problem
 5 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
 6 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
 0 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