checkCIF/PLATON report

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

Datablock: sw144

Bond precision: C-C = 0.0116 A   Wavelength=1.54178

Cell:	a=11.1795(3)	b=12.7224(3)	c=19.4919(6)
	alpha=101.365(2)	beta=90.710(2)	gamma=109.057(2)

Temperature: 123 K

	Calculated	Reported
Volume	2560.19(13)	2560.19(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C45 H41 Cu2 Mo2 N3 O4 P4, 2(B F4)	C45 H41 Cu2 Mo2 N3 O4 P4, 2(B F4)
Sum formula	C45 H41 B2 Cu2 F8 Mo2 N3 O4 P4	C45 H41 B2 Cu2 F8 Mo2 N3 O4 P4
Mr	1304.29	1304.29
Dx,g cm-3	1.692	1.692
Z	2	2
Mu (mm-1)	6.682	6.682
F000	1296.0	1296.0
F000'	1293.49	
h,k,lmax	12,14,22	12,14,22
Nref	8135	7802
Tmin,Tmax	0.402,0.544	0.274,0.609
Tmin'	0.111	

Correction method= ANALYTICAL

Data completeness= 0.959   Theta(max)= 62.380

R(reflections)= 0.0537(6952)   wR2(reflections)= 0.1618(7802)

S = 1.059   Npar= 631

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 B**
THETM01_ALERT_3_B   The value of sine(theta_max)/wavelength is less than 0.575
           Calculated sin(theta_max)/wavelength =   0.5747
PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full Low 0.96
PLAT220_ALERT_2_B Large Non-Solvent   C   Ueq(max)/Ueq(min) ...   4.11 Ratio

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PLAT222_ALERT_3_B Large Non-Solvent    H    Ueq(max)/Ueq(min) ...        5.00 Ratio
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Alert level C
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DIFMX01_ALERT_2_C  The maximum difference density is > 0.1*ZMAX*0.75
            _refine_diff_density_max given =      3.631
            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.
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density      3.63 eA-3
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds (x 1000) Ang ..       12
PLAT432_ALERT_2_C Short Inter X...Y Contact  F11    ..  C42    ..      2.91 Ang.
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of       B2
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of       B3
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Alert level G
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PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large..      0.10
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.     10.57
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......      374
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal  (x 10000)      200 Deg.
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................    33.00 Perc.
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   0 ALERT level A = In general: serious problem
   4 ALERT level B = Potentially serious problem
   7 ALERT level C = Check and explain
   5 ALERT level G = General alerts; check

   2 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
   5 ALERT type 3 Indicator that the structure quality may be low
   3 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