

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw272

Bond precision: C-C = 0.0114 A Wavelength=1.54178

Cell: a=12.5970(6) b=13.6463(7) c=14.4682(7)
 alpha=81.688(4) beta=67.192(5) gamma=67.492(4)

Temperature: 123 K

	Calculated	Reported
Volume	2118.0(2)	2118.0(2)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C56 H40 Cu2 Mo8 O16 P8, 4(C H2 Cl2), 2(B F4)	C56 H40 Cu2 Mo8 O16 P8, 4(C H2 Cl2), 2(B F4)
Sum formula	C60 H48 B2 Cl8 Cu2 F8 Mo8 O16 P8	C60 H48 B2 Cl8 Cu2 F8 Mo8 O16 P8
Mr	2624.59	2624.59
Dx,g cm-3	2.058	2.058
Z	1	1
Mu (mm-1)	14.309	14.309
F000	1268.0	1268.0
F000'	1271.43	
h,k,lmax	13,15,16	13,15,16
Nref	6073	6036
Tmin,Tmax	0.127,0.251	0.257,1.000
Tmin'	0.005	

Correction method= MULTI-SCAN

Data completeness= 0.994 Theta(max)= 58.930

R(reflections)= 0.0396(5113) wR2(reflections)= 0.1088(6036)

S = 1.026 Npar= 505

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 = 0.5556

● Alert level C

PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Mo1	--	C11	..	6.31	su
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds (x 1000) Ang	..			11	
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of				C2S	
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of				B1	

● Alert level G

PLAT432_ALERT_2_G	Short Inter X...Y Contact	C12	..	C23	..	3.25	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C5	..	C20	..	3.20	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact	C7	..	C7	..	3.16	Ang.
PLAT720_ALERT_4_G	Number of Unusual/Non-Standard Labels				4	

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

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

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 31/03/2010; check.def file version of 22/03/2010

