

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw270

Bond precision: C-C = 0.0205 A Wavelength=1.54178

Cell: a=9.9741(1) b=33.8250(3) c=17.7309(1)
 alpha=90 beta=94.134(1) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	5966.38(9)	5966.38(9)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C24 H30 Cu Mo2 O4 P6, C16 Al F36 O4	C24 H30 Cu Mo2 O4 P6, C16 Al F36 O4
Sum formula	C40 H30 Al Cu F36 Mo2 O8 P6	C40 H30 Al Cu F36 Mo2 O8 P6
Mr	1790.87	1790.87
Dx,g cm-3	1.994	1.994
Z	4	4
Mu (mm-1)	6.982	6.982
F000	3496.0	3496.0
F000'	3510.23	
h,k,lmax	11,39,20	11,39,20
Nref	10171	10132
Tmin,Tmax	0.276,0.735	0.238,0.737
Tmin'	0.040	

Correction method= ANALYTICAL

Data completeness= 0.996 Theta(max)= 65.080

R(reflections)= 0.1020(9606) wR2(reflections)= 0.2574(10132)

S = 1.100 Npar= 1009

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

PLAT241_ALERT_2_B Check High	Ueq as Compared to Neighbors for	O8
PLAT242_ALERT_2_B Check Low	Ueq as Compared to Neighbors for	All
PLAT242_ALERT_2_B Check Low	Ueq as Compared to Neighbors for	C300
PLAT242_ALERT_2_B Check Low	Ueq as Compared to Neighbors for	C400

PLAT242_ALERT_2_B	Check Low	Ueq as Compared to Neighbors for	C401
PLAT242_ALERT_2_B	Check Low	Ueq as Compared to Neighbors for	C403
PLAT234_ALERT_4_B	Large Hirshfeld Difference F4A	-- C10B ..	0.26 Ang.
PLAT234_ALERT_4_B	Large Hirshfeld Difference F32	-- C402 ..	0.27 Ang.

● **Alert level C**

RFACG01_ALERT_3_C	The value of the R factor is > 0.10		
	R factor given	0.102	
RFACR01_ALERT_3_C	The value of the weighted R factor is > 0.25		
	Weighted R factor given	0.257	
THETM01_ALERT_3_C	The value of sine(theta_max)/wavelength is less than 0.590		
	Calculated sin(theta_max)/wavelength =	0.5882	
PLAT084_ALERT_2_C	High wR2 Value		0.26
PLAT213_ALERT_2_C	Atom C18B	has ADP max/min Ratio	3.20 prola
PLAT213_ALERT_2_C	Atom C18	has ADP max/min Ratio	3.20 prola
PLAT213_ALERT_2_C	Atom C20	has ADP max/min Ratio	3.70 prola
PLAT213_ALERT_2_C	Atom F13	has ADP max/min Ratio	3.40 prola
PLAT213_ALERT_2_C	Atom F16	has ADP max/min Ratio	3.10 prola
PLAT213_ALERT_2_C	Atom F30	has ADP max/min Ratio	3.10 prola
PLAT213_ALERT_2_C	Atom F31	has ADP max/min Ratio	3.10 prola
PLAT213_ALERT_2_C	Atom O6	has ADP max/min Ratio	3.20 prola
PLAT220_ALERT_2_C	Large Non-Solvent	C Ueq(max)/Ueq(min) ...	3.59 Ratio
PLAT220_ALERT_2_C	Large Non-Solvent	F Ueq(max)/Ueq(min) ...	3.10 Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	F12 -- C201 ..	5.37 su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1 -- P5 ..	7.13 su
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	06
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for	07
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C100
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C202
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C203
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C302
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds (x 1000) Ang ..	20
PLAT142_ALERT_4_C	su on b - Axis Small or Missing	(x 100000)	30 Ang.
PLAT143_ALERT_4_C	su on c - Axis Small or Missing	(x 100000)	10 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F3A	-- C10A ..	0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F8A	-- C10C ..	0.24 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F10	-- C201 ..	0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F15	-- C202 ..	0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F20	-- C301 ..	0.22 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F21	-- C301 ..	0.20 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F27	-- C303 ..	0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F31	-- C402 ..	0.21 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference O8	-- C400 ..	0.15 Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C400	-- C403 ..	0.17 Ang.

● **Alert level G**

PLAT072_ALERT_2_G	SHELXL First Parameter in WGHT Unusually Large.	0.10
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	96.99
PLAT301_ALERT_3_G	Note: Main Residue Disorder	20.00 Perc.
PLAT432_ALERT_2_G	Short Inter X...Y Contact F36 .. C22B ..	2.78 Ang.
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	564
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	!

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
28 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
14 ALERT type 4 Improvement, methodology, query or suggestion
1 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 29/06/2010; check.def file version of 26/06/2010

Datablock sw270 - ellipsoid plot

