

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw257

Bond precision: C-C = 0.0058 A Wavelength=1.54178

Cell: a=16.2779(1) b=11.2983(1) c=31.1713(3)
 alpha=90 beta=119.808(1) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	4974.33(9)	4974.33(9)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C28 H20 Cu2 Mo4 O8 P12, 2(C16 Al F36 O4)	C28 H20 Cu2 Mo4 O8 P12, 2(C16 Al F36 O4)
Sum formula	C60 H20 Al2 Cu2 F72 Mo4 O16 P12	C60 H20 Al2 Cu2 F72 Mo4 O16 P12
Mr	3301.22	3301.22
Dx,g cm-3	2.204	2.204
Z	2	2
Mu (mm-1)	8.301	8.301
F000	3176.0	3176.0
F000'	3189.57	
h,k,lmax	20,14,38	20,14,38
Nref	9974	9836
Tmin,Tmax	0.230,0.411	0.092,0.486
Tmin'	0.002	

Correction method= ANALYTICAL

Data completeness= 0.986 Theta(max)= 73.200

R(reflections)= 0.0373(9598) wR2(reflections)= 0.1026(9836)

S = 1.074 Npar= 757

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

PLAT213_ALERT_2_B Atom C9 has ADP max/min Ratio 4.30 prola

● Alert level C

PLAT213_ALERT_2_C	Atom C1	has ADP max/min Ratio	3.70	prola
PLAT213_ALERT_2_C	Atom C2	has ADP max/min Ratio	3.10	prola
PLAT220_ALERT_2_C	Large Non-Solvent	C Ueq(max)/Ueq(min) ...	3.15	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	F14 -- C202 ..	5.43	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo1 -- P1 ..	6.41	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo1 -- P3 ..	5.03	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo1 -- C6 ..	6.97	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo1 -- C7 ..	6.67	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo2 -- P4 ..	5.89	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo2 -- P6 ..	5.13	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo2 -- C13 ..	5.54	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo2 -- C14 ..	6.28	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1 -- P1 ..	5.79	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1 -- P4 ..	6.25	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1 -- P5 ..	7.33	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1 -- P1_a ..	5.92	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1 -- P3_a ..	5.16	su
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for		C9
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for		Mo2
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j)	Tensor	2.06	
PLAT431_ALERT_2_C	Short Inter HL..A Contact	F2 .. O4 ..	2.84	Ang.
PLAT432_ALERT_2_C	Short Inter X...Y Contact	P4 .. P6 ..	3.38	Ang.
PLAT141_ALERT_4_C	su on a - Axis Small or Missing (x 100000)	10	Ang.
PLAT142_ALERT_4_C	su on b - Axis Small or Missing (x 100000)	10	Ang.
PLAT143_ALERT_4_C	su on c - Axis Small or Missing (x 100000)	30	Ang.

● Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	8.77	
PLAT063_ALERT_4_G	Crystal Size Likely too Large for Beam Size	0.72	mm
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P6	

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

- 0 **ALERT type 1** CIF construction/syntax error, inconsistent or missing data
 - 24 **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
 - 5 **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

Datablock sw257 - ellipsoid plot

