

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw256II

Bond precision: C-C = 0.0054 Å Wavelength=1.54178

Cell: a=13.4258(1) b=7.3930(1) c=19.6321(2)
 alpha=90 beta=126.611(1) gamma=90

Temperature: 123 K

	Calculated	Reported
Volume	1564.17(4)	1564.17(4)
Space group	P 2/c	P 2/c
Hall group	-P 2yc	-P 2yc
Moiety formula	C14 H10 Mo2 O4 P2	C14 H10 Mo2 O4 P2
Sum formula	C14 H10 Mo2 O4 P2	C14 H10 Mo2 O4 P2
Mr	496.04	496.04
Dx, g cm ⁻³	2.106	2.106
Z	4	4
Mu (mm ⁻¹)	15.201	15.201
F000	960.0	960.0
F000'	963.73	
h,k,lmax	16,9,23	16,9,23
Nref	2972	2970
Tmin,Tmax	0.021,0.050	0.039,0.222
Tmin'	0.003	

Correction method= GAUSSIAN

Data completeness= 0.999 Theta(max)= 70.070

R(reflections)= 0.0276(2955) wR2(reflections)= 0.0740(2970)

S = 1.169 Npar= 200

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

PLAT230_ALERT_2_B	Hirshfeld Test Diff for	O2	--	C7	..	7.89	su
PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Mo1	--	C7	..	10.06	su

Alert level C

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O3	--	C13	..	5.55	su
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PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo2	--	C13	..	7.95	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo2	--	C14	..	6.05	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo2	--	P2_b	..	5.07	su
PLAT141_ALERT_4_C	su on a - Axis Small or Missing (x 100000)				10	Ang.

● **Alert level G**

PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P1
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.	P2

0 **ALERT level A** = In general: serious problem
2 **ALERT level B** = Potentially serious problem
5 **ALERT level C** = Check and explain
2 **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
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 13/08/2009; check.def file version of 12/08/2009

