

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw248

Bond precision: C-C = 0.0106 Å

Wavelength=1.54178

Cell: a=9.2107(5) b=12.3099(6) c=12.4871(6)
 alpha=87.582(4) beta=75.331(4) gamma=83.746(4)
Temperature: 123 K

	Calculated	Reported
Volume	1361.37(12)	1361.37(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C26 H34 Mo2 O4 P2	C26 H34 Mo2 O4 P2
Sum formula	C26 H34 Mo2 O4 P2	C26 H34 Mo2 O4 P2
Mr	664.35	664.35
Dx, g cm ⁻³	1.621	1.621
Z	2	2
Mu (mm ⁻¹)	8.893	8.893
F000	672.0	672.0
F000'	674.23	
h,k,lmax	10,14,14	10,14,14
Nref	4492	4428
Tmin,Tmax	0.392,0.847	0.462,0.846
Tmin'	0.246	

Correction method= ANALYTICAL

Data completeness= 0.986

Theta(max)= 63.680

R(reflections)= 0.0550(4086)

wR2(reflections)= 0.1295(4428)

S = 1.060

Npar= 317

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

DIFMX01_ALERT_2_B The maximum difference density is > 0.1*ZMAX*1.00

 _refine_diff_density_max given = 5.610

 Test value = 4.200

PLAT097_ALERT_2_B Large Reported Max. (Positive) Residual Density 5.61 eA-3

● Alert level C

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590
Calculated sin(theta_max)/wavelength = 0.5814

PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 3.09

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.18 Ratio

PLAT222_ALERT_3_C Large Non-Solvent H Ueq(max)/Ueq(min) ... 3.88 Ratio

PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo2 -- P1 .. 6.48 su

PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo2 -- P2 .. 5.88 su

PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo2 -- C4 .. 5.63 su

PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C21

PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang .. 11

● Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 14.59

PLAT154_ALERT_1_G The su's on the Cell Angles are Equal (x 10000) 400 Deg.

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

10 **ALERT level C** = Check and explain

4 **ALERT level G** = General alerts; check

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

9 ALERT type 2 Indicator that the structure model may be wrong or deficient

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

2 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

