

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw220

Bond precision: C-C = 0.0040 Å Wavelength=1.54178

Cell: a=15.8694(11) b=14.6679(10) c=15.9594(12)
 alpha=90 beta=102.587(7) gamma=90

Temperature: 101 K

	Calculated	Reported
Volume	3625.6(5)	3625.6(5)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C13 H15 Fe Mo O3 P5	C13 H15 Fe Mo O3 P5
Sum formula	C13 H15 Fe Mo O3 P5	C13 H15 Fe Mo O3 P5
Mr	525.89	525.89
Dx, g cm ⁻³	1.927	1.927
Z	8	8
Mu (mm ⁻¹)	16.348	16.348
F000	2080.0	2080.0
F000'	2085.93	
h,k,lmax	18,17,19	18,17,18
Nref	3214	3185
Tmin,Tmax	0.179,0.303	0.153,0.303
Tmin'	0.027	

Correction method= MULTI-SCAN

Data completeness= 0.991 Theta(max)= 66.750

R(reflections)= 0.0237(3001) wR2(reflections)= 0.0699(3185)

S = 1.076 Npar= 213

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 C

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	O2	--	C12	..	6.08	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo1	--	P5	..	6.74	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo1	--	C11	..	6.28	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo1	--	C12	..	8.36	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Mo1	--	C13	..	7.12	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe1	--	P2	..	6.35	su

PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe1	--	P3	..	6.60	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe1	--	P4	..	6.62	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe1	--	P5	..	5.40	su
PLAT380_ALERT_4_C	Check Incorrectly? Oriented X(sp2)-Methyl Moiety						C6

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

0 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
 0 ALERT type 3 Indicator that the structure quality may be low
 1 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 09/04/2009; check.def file version of 08/04/2009

