checkCIF/PLATON report

No syntax errors found.　　　CIF dictionary　　　Interpreting this report

Datablock: sw258

Bond precision:　C-C = 0.0060 A　　　　　Wavelength=1.54178

Cell:　　　　　　a=8.7702(1)　　　b=26.5995(3)　　　c=19.5513(3)
　　　　　　　　　alpha=90　　　　　beta=116.205(1)　　gamma=90
Temperature:　　123 K

	Calculated	Reported
Volume	4092.21(10)	4092.21(10)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C26 H30 Ag B F4 Fe2 Mo2 O6 P10	C26 H30 Ag B F4 Fe2 Mo2 O6 P10
Sum formula	C26 H30 Ag B F4 Fe2 Mo2 O6 P10	C26 H30 Ag B F4 Fe2 Mo2 O6 P10
Mr	1246.46	1246.46
Dx,g cm-3	2.023	2.023
Z	4	4
Mu (mm-1)	18.417	18.417
F000	2432.0	2432.0
F000'	2440.03	
h,k,lmax	10,32,23	10,32,23
Nref	7781	7769
Tmin,Tmax	0.065,0.112	0.081,0.276
Tmin'	0.005	

Correction method= ANALYTICAL

Data completeness= 0.998　　　　　Theta(max)= 70.090

R(reflections)= 0.0355(7380)　　　wR2(reflections)= 0.0949(7769)

S = 1.103　　　　　　　　Npar= 479

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**
DIFMX01_ALERT_2_C　The maximum difference density is > 0.1*ZMAX*0.75
　　　　_refine_diff_density_max given =　　3.703
　　　　Test value =　　3.525
DIFMX02_ALERT_1_C　The maximum difference density is > 0.1*ZMAX*0.75

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                The relevant atom site should be identified.
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....     3.66
PLAT097_ALERT_2_C Large Reported Max.  (Positive) Residual Density      3.70 eA-3
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O1    -- C11    ..         5.77 su
PLAT230_ALERT_2_C Hirshfeld Test Diff for    O5    -- C25    ..         5.21 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo1   -- P1     ..          5.39 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo1   -- P2     ..          6.86 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo1   -- P3     ..          7.17 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo1   -- P4     ..          6.71 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo1   -- C11    ..          8.06 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo1   -- C13    ..          5.46 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo2   -- P6     ..          6.00 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo2   -- P7     ..          8.62 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo2   -- P8     ..          7.14 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo2   -- P9     ..          6.71 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo2   -- P10    ..          5.38 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo2   -- C24    ..          5.72 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo2   -- C25    ..          6.53 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mo2   -- C26    ..          5.60 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Fe1   -- P2     ..          6.28 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Fe1   -- P4     ..          5.54 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Fe2   -- P6     ..          5.31 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Fe2   -- P7     ..          7.24 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Fe2   -- P8     ..          6.96 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Fe2   -- P9     ..          5.95 su
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for      F1
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for      B1
PLAT413_ALERT_2_C Short Inter XH3 .. XHn     H7A    .. H7A    ..        2.13 Ang.
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⬤ **Alert level G**
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PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.      5.84
PLAT380_ALERT_4_G Check Incorrectly? Oriented X(sp2)-Methyl Moiety      C6
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   0 ALERT level A = In general: serious problem
   0 ALERT level B = Potentially serious problem
  29 ALERT level C = Check and explain
   2 ALERT level G = General alerts; check

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  29 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
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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 sw258 - ellipsoid plot