

# checkCIF/PLATON report

No syntax errors found.      CIF dictionary      Interpreting this report

**Datablock: sw246**

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Bond precision:	C-C = 0.0113 A	Wavelength=1.54178	
Cell:	a=19.6554(16)	b=9.6564(9)	c=36.745(3)
	alpha=90	beta=98.912(9)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	6890.0(10)	6890.0(10)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C26 H30 Ag Fe2 Mo2 O6 P10, C16 Al F36 O4	C26 H30 Ag Fe2 Mo2 O6 P10, C16 Al F36 O4	
Sum formula	C42 H30 Ag Al F36 Fe2 Mo2 O10 P10	C42 H30 Ag Al F36 Fe2 Mo2 O10 P10	
Mr	2126.79	2126.79	
Dx,g cm-3	2.050	2.050	
Z	4	4	
Mu (mm-1)	12.144	12.144	
F000	4128.0	4128.0	
F000'	4147.52		
h,k,lmax	23,11,43	23,11,43	
Nref	12173	12100	
Tmin,Tmax	0.097,0.762	0.232,1.000	
Tmin'	0.011		

Correction method= MULTI-SCAN

Data completeness= 0.994      Theta(max)= 66.590

R(reflections)= 0.0520( 10079)      wR2(reflections)= 0.1875( 12100)

S = 1.153      Npar= 947

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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.

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## Alert level C

PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for	C80
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds (x 1000) Ang ..	11
PLAT432_ALERT_2_C	Short Inter X...Y Contact	F4 .. C1 ..	2.92 Ang.
PLAT432_ALERT_2_C	Short Inter X...Y Contact	F12 .. C15 ..	2.91 Ang.

PLAT601_ALERT_2_C	Structure Contains Solvent Accessible Voids of .	36.00	A**3
PLAT234_ALERT_4_C	Large Hirshfeld Difference F10 -- C81 ..	0.15	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference F17 -- C83 ..	0.16	Ang.



#### Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.	69.84
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0	ALERT level A	= In general: serious problem
0	ALERT level B	= Potentially serious problem
7	ALERT level C	= Check and explain
1	ALERT level G	= General alerts; check

  

0	ALERT type 1	CIF construction/syntax error, inconsistent or missing data
5	ALERT type 2	Indicator that the structure model may be wrong or deficient
1	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

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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.

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PLATON version of 13/08/2009; check.def file version of 12/08/2009

