

# checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

## Datablock: swr16

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Bond precision: C-C = 0.0140 Å Wavelength=0.71073  
Cell: a=21.779(2) b=13.0427(10) c=25.1275(17)  
alpha=90 beta=120.057(5) gamma=90  
Temperature: 100 K

	Calculated	Reported
Volume	6177.8(9)	6177.8(9)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C54 H51 B Cu3 F4 Mo2 N4 O4 P5, 2(B F4)	C54 H51 B Cu3 F4 Mo2 N4 O4 P5, 2(B F4)
Sum formula	C54 H51 B3 Cu3 F12 Mo2 N4 O4 P5	C54 H51 B3 Cu3 F12 Mo2 N4 O4 P5
Mr	1617.80	1617.80
Dx,g cm-3	1.739	1.739
Z	4	4
Mu (mm-1)	1.624	1.624
F000	3216.0	3216.0
F000'	3209.46	
h,k,lmax	27,16,31	27,16,31
Nref	12897	12668
Tmin,Tmax	0.925,0.984	0.369,0.984
Tmin'	0.723	

Correction method= MULTI-SCAN

Data completeness= 0.982 Theta(max)= 26.560

R(reflections)= 0.0553( 6826) wR2(reflections)= 0.1534( 12668)

S = 0.972 Npar= 788

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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 A

PLAT220\_ALERT\_2\_A Large Non-Solvent C Ueq(max)/Ueq(min) ... 6.05 Ratio

**Author Response: The thermal movement of the terminal acetonitrile ligands is stronger compared to the other C and H containing moieties.**

PLAT222\_ALERT\_3\_A Large Non-Solvent H Ueq(max)/Ueq(min) ... 7.86 Ratio

**Author Response: The thermal movement of the terminal acetonitrile ligands is stronger compared to the other C and H containing moieties.**

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● **Alert level C**

PLAT213_ALERT_2_C	Atom C512	has ADP max/min Ratio .....	3.80	prola
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Mol	-- C300 ..	5.02	su
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for		C24
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for		Cu1
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for		C501
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for		B3
PLAT331_ALERT_2_C	Small Average Phenyl	C-C Dist. C10 -C15	1.36	Ang.
PLAT331_ALERT_2_C	Small Average Phenyl	C-C Dist. C20 -C25	1.37	Ang.
PLAT342_ALERT_3_C	Low Bond Precision on	C-C Bonds (x 1000) Ang ..		14
PLAT432_ALERT_2_C	Short Inter X...Y Contact	F20 .. C511 ..	2.91	Ang.
PLAT432_ALERT_2_C	Short Inter X...Y Contact	F20 .. C501 ..	2.91	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	F33 -- B3 ..	0.23	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	O300 -- C300 ..	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C10 -- C11 ..	0.16	Ang.
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of			B1

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● **Alert level G**

PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints .....	60
PLAT793_ALERT_4_G	The Model has Chirality at P2 (Verify) ....	R

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2 **ALERT level A** = In general: serious problem

0 **ALERT level B** = Potentially serious problem

15 **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

11 **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

5 **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

Datablock swr16 - ellipsoid plot

