

# checkCIF/PLATON report

No syntax errors found.    CIF dictionary    Interpreting this report

## Datablock: sw194

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Bond precision:    C-C = 0.0132 A                      Wavelength=1.54178  
Cell:                      a=17.5130(3)              b=21.7843(3)              c=32.5894(4)  
                            alpha=90                      beta=90                      gamma=90  
Temperature:              105 K

	Calculated	Reported
Volume	12433.1(3)	12433.1(3)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C40 H60 Cu2 Fe4 P20	C40 H60 Cu2 Fe4 P20
Sum formula	C40 H60 Cu2 Fe4 P20	C40 H60 Cu2 Fe4 P20
Mr	1510.78	1510.78
Dx,g cm-3	0.807	0.807
Z	4	4
Mu (mm-1)	6.569	6.569
F000	3048.0	3048.0
F000'	3041.61	
h,k,lmax	19,24,36	19,24,36
Nref	10046[ 18482]	18417
Tmin,Tmax	0.217,0.308	
Tmin'	0.019	

Correction method= Not given

Data completeness= 1.83/1.00                      Theta(max)= 60.020

R(reflections)= 0.0682( 16105)                      wR2(reflections)= 0.1903( 18417)

S = 1.076    Npar= 573

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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 B

THETM01\_ALERT\_3\_B The value of sine(theta\_max)/wavelength is less than 0.575

Calculated sin(theta\_max)/wavelength = 0.5618

PLAT241_ALERT_2_B	Check High	Ueq as Compared to Neighbors for	C23
PLAT049_ALERT_1_B	Calculated Density less than 1.0 gcm-3	.....	0.81
PLAT234_ALERT_4_B	Large Hirshfeld Difference	C21 -- C22 ..	0.26 Ang.
PLAT234_ALERT_4_B	Large Hirshfeld Difference	C23 -- C24 ..	0.22 Ang.

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**Alert level C**

PLAT220_ALERT_2_C	Large Non-Solvent	C	Ueq(max)/Ueq(min) ...	3.19	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C11	-- C16 ..	5.04	su
PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C22	-- C23 ..	6.58	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1	-- P11 ..	5.85	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu2	-- P2 ..	5.78	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe1	-- P2 ..	6.84	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe1	-- C2 ..	5.70	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe2	-- C15 ..	5.34	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe3	-- P13 ..	8.11	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe3	-- P15 ..	5.76	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe4	-- P20 ..	8.35	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe4	-- C33 ..	5.72	su
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for			P4
PLAT241_ALERT_2_C	Check High	Ueq as Compared to Neighbors for			P5
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for			Fe1
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for			Fe3
PLAT242_ALERT_2_C	Check Low	Ueq as Compared to Neighbors for			C24
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds (x 1000)	Ang	...	13	
PLAT234_ALERT_4_C	Large Hirshfeld Difference	Fe1	-- C3 ..	0.12	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	Fe1	-- C5 ..	0.10	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	Fe2	-- C13 ..	0.14	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	Fe3	-- C21 ..	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	Fe3	-- C23 ..	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	Fe3	-- C24 ..	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	Fe3	-- C25 ..	0.18	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	Fe4	-- C32 ..	0.13	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C1	-- C2 ..	0.14	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C1	-- C5 ..	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C1	-- C6 ..	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C2	-- C7 ..	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C3	-- C4 ..	0.12	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C3	-- C8 ..	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C4	-- C9 ..	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C13	-- C18 ..	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C14	-- C19 ..	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C31	-- C35 ..	0.14	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C31	-- C36 ..	0.15	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference	C34	-- C35 ..	0.14	Ang.
PLAT328_ALERT_4_C	Check for Possibly Missing H on sp3?	Phosphorus.			P3
PLAT328_ALERT_4_C	Check for Possibly Missing H on sp3?	Phosphorus.			P4
PLAT328_ALERT_4_C	Check for Possibly Missing H on sp3?	Phosphorus.			P5
PLAT328_ALERT_4_C	Check for Possibly Missing H on sp3?	Phosphorus.			P8
PLAT328_ALERT_4_C	Check for Possibly Missing H on sp3?	Phosphorus.			P9
PLAT328_ALERT_4_C	Check for Possibly Missing H on sp3?	Phosphorus.			P10
PLAT328_ALERT_4_C	Check for Possibly Missing H on sp3?	Phosphorus.			P13
PLAT328_ALERT_4_C	Check for Possibly Missing H on sp3?	Phosphorus.			P14
PLAT328_ALERT_4_C	Check for Possibly Missing H on sp3?	Phosphorus.			P15
PLAT328_ALERT_4_C	Check for Possibly Missing H on sp3?	Phosphorus.			P17
PLAT328_ALERT_4_C	Check for Possibly Missing H on sp3?	Phosphorus.			P18
PLAT328_ALERT_4_C	Check for Possibly Missing H on sp3?	Phosphorus.			P20
PLAT380_ALERT_4_C	Check Incorrectly? Oriented X(sp2)-Methyl Moiety				C8

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**Alert level G**

REFLT03\_ALERT\_4\_G Please check that the estimate of the number of Friedel pairs is correct. If it is not, please give the correct count in the `_publ_section_exptl_refinement` section of the submitted CIF.

From the CIF: `_diffrn_reflns_theta_max` 60.02  
From the CIF: `_reflns_number_total` 18417  
Count of symmetry unique reflns 10046

Completeness (\_total/calc) 183.33%  
TEST3: Check Friedels for noncentro structure  
Estimate of Friedel pairs measured 8371  
Fraction of Friedel pairs measured 0.833  
Are heavy atom types Z>Si present yes  
PLAT860\_ALERT\_3\_G Note: Number of Least-Squares Restraints ..... 6  
PLAT606\_ALERT\_4\_G VERY LARGE Solvent Accessible VOID(S) in Structure !

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
18 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  
37 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 12/11/2008; check.def file version of 12/11/2008**

# Datablock sw194 - ellipsoid plot

