

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw194

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

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 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.



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



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: _diffn_reflns_theta_max 60.02

From the CIF: _reflns_number_total 18417

Count of symmetry unique reflns 10046

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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.

PLATON version of 12/11/2008; check.def file version of 12/11/2008

Datablock sw194 - ellipsoid plot

