

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw164

Bond precision: C-C = 0.0026 Å Wavelength=0.71073

Cell: a=12.0416(1) b=12.0416(1) c=21.5976(4)
 alpha=90 beta=90 gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	3131.66(7)	3131.66(7)
Space group	P -4 21 c	P -4 21 c
Hall group	P -4 2n	P -4 2n
Moiety formula	C10 H15 Cl Cu Fe P5	C10 H15 Cl Cu Fe P5
Sum formula	C10 H15 Cl Cu Fe P5	C10 H15 Cl Cu Fe P5
Mr	444.92	444.92
Dx, g cm ⁻³	1.887	1.887
Z	8	8
Mu (mm ⁻¹)	2.943	2.943
F000	1776.0	1776.0
F000'	1786.73	
h,k,lmax	18,18,33	18,18,33
Nref	3448[6265]	6225
Tmin,Tmax	0.320,0.649	0.374,0.649
Tmin'	0.183	

Correction method= MULTI-SCAN

Data completeness= 1.81/0.99 Theta(max)= 33.730

R(reflections)= 0.0256(5664) wR2(reflections)= 0.0594(6225)

S = 1.040 Npar= 168

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

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Cu1 -- P4_b .. 12.41 su



Alert level C

PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu1 -- P1 .. 7.26 su

PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Cu1 -- P2_a .. 8.87 su

```
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Fe1 -- P3 .. 6.18 su
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Fe1 -- P5 .. 5.87 su
PLAT141_ALERT_4_C su on a - Axis Small or Missing (x 100000) ..... 10 Ang.
```

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_reflths_theta_max 33.73

From the CIF: _reflns_number_total 6225

Count of symmetry unique reflns 3448

Completeness (_total/calc) 180.54%

TEST3: Check Friedels for noncentro structure

Estimate of Friedel pairs measured 2777

Fraction of Friedel pairs measured 0.805

Are heavy atom types Z>Si present yes

PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus. P3

PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus. P5

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

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

5 **ALERT level C** = Check and explain

3 **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

0 ALERT type 3 Indicator that the structure quality may be low

4 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

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 31/03/2010; check.def file version of 22/03/2010

