checkCIF/PLATON report

No syntax errors found.   CIF dictionary   Interpreting this report

Datablock: sw240

Bond precision: C-C = 0.0042 A   Wavelength=1.54178

Cell: a=14.3882(3)   b=15.8072(3)   c=22.5059(5)
                alpha=91.063(2)   beta=93.522(2)   gamma=91.974(2)
Temperature: 123 K

	Calculated	Reported
Volume	5104.88(18)	5104.88(18)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C34 H37 Cu2 Fe N6 P5), 5(C H2 Cl2), 4(B F4)	2(C34 H37 Cu2 Fe N6 P5), 5(C H2 Cl2), 4(B F4)
Sum formula	C73 H84 B4 Cl10 Cu4 F16 Fe2 N12 P10	C73 H84 B4 Cl10 Cu4 F16 Fe2 N12 P10
Mr	2506.86	2506.86
Dx,g cm-3	1.631	1.631
Z	2	2
Mu (mm-1)	7.675	7.675
F000	2516.0	2516.0
F000'	2514.66	
h,k,lmax	17,18,26	17,18,26
Nref	18071	17818
Tmin,Tmax	0.117,0.312	0.237,0.523
Tmin'	0.032	

Correction method= ANALYTICAL

Data completeness= 0.986   Theta(max)= 66.720

R(reflections)= 0.0448(15278)   wR2(reflections)= 0.1324(17818)

S = 1.066   Npar= 1311

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
PLAT431_ALERT_2_B Short Inter HL..A Contact Cl9   .. Cl8B   ..   3.10 Ang.

Alert level C

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PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X)  Fe2    --  P9       ..      5.24 su
PLAT432_ALERT_2_C Short Inter X...Y Contact  F6B    ..  C43      ..      2.87 Ang.
PLAT432_ALERT_2_C Short Inter X...Y Contact  F9B    ..  C65      ..      2.93 Ang.
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        C2S
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        C3S
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        C5S
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        B1
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        B2B
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        B3B
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        B4
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        C4SB
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        B2A
PLAT244_ALERT_4_C Low   'Solvent' Ueq as Compared to Neighbors of        B3A
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Alert level G

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PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints .......     211
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal  (x 10000)     200 Deg.
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder ...................   27.00 Perc.
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.      P4
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      P5
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      P8
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      P9
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      P10
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........      14
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  0 ALERT level A = In general: serious problem
  1 ALERT level B = Potentially serious problem
 13 ALERT level C = Check and explain
 10 ALERT level G = General alerts; check

  1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  4 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
 18 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 13/08/2009; check.def file version of 12/08/2009

NOMOVE FORCED

Prob = 50
Temp = 123

32 Y

PLATON-Oct 26 21:16:40 2009 - (130809)

Z -83   sw240   P -1   R = 0.04   RES=   0   -10 X