

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw265

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

Cell: a=13.0690(3) b=14.0653(4) c=14.5466(4)
 alpha=81.484(2) beta=88.927(2) gamma=77.420(2)

Temperature: 123 K

	Calculated	Reported
Volume	2580.73(12)	2580.73(12)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C80 H74 Cu4 N12 P2, 4(B F4)	C80 H74 Cu4 N12 P2, 4(B F4)
Sum formula	C80 H74 B4 Cu4 F16 N12 P2	C80 H74 B4 Cu4 F16 N12 P2
Mr	1866.89	1866.89
Dx,g cm-3	1.201	1.201
Z	1	1
Mu (mm-1)	1.825	1.825
F000	948.0	948.0
F000'	943.56	
h,k,lmax	16,17,18	16,17,18
Nref	10446	10021
Tmin,Tmax	0.803,0.902	0.537,0.783
Tmin'	0.756	

Correction method= ANALYTICAL

Data completeness= 0.959 Theta(max)= 73.800

R(reflections)= 0.0466(8446) wR2(reflections)= 0.1317(10021)

S = 1.118 Npar= 702

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

PLAT029_ALERT_3_B _diffn_measured_fraction_theta_full Low 0.96

Alert level C

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.53 Ratio

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	N6	--	C39	..	5.59	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1	--	N5	..	5.99	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu2	--	P1	..	7.56	su
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						B2

● **Alert level G**

PLAT301_ALERT_3_G	Note: Main Residue Disorder	22.00	Perc.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C37 .. F3B ..	2.89	Ang.
PLAT432_ALERT_2_G	Short Inter X...Y Contact C38 .. F3B ..	2.86	Ang.
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints	138	
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	37.00	Perc.
PLAT606_ALERT_4_G	VERY LARGE Solvent Accessible VOID(S) in Structure		!
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms		!

0 **ALERT level A** = In general: serious problem
1 **ALERT level B** = Potentially serious problem
6 **ALERT level C** = Check and explain
8 **ALERT level G** = General alerts; check

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 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
4 ALERT type 4 Improvement, methodology, query or suggestion
1 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

