

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: sw163

Bond precision: C-C = 0.0123 A Wavelength=1.54178

Cell: a=21.3242(1) b=26.9244(2) c=33.3967(2)
 alpha=90 beta=90.508(1) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	19173.7(2)	19173.7(2)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C90 H135 Cl10 Cu10 Fe9 P45, C10 H15 Fe P5, 2(C7 H8)	C90 H135 Cl10 Cu10 Fe9 P45, C10 H15 Fe P5, 2(C7 H8)
Sum formula	C114 H166 Cl10 Cu10 Fe10 P50	C114 H166 Cl10 Cu10 Fe10 P50
Mr	4633.47	4633.47
Dx,g cm-3	1.605	1.605
Z	4	4
Mu (mm-1)	12.548	12.548
F000	9280.0	9280.0
F000'	9240.48	
h,k,lmax	24,30,38	24,30,38
Nref	30306	28827
Tmin,Tmax	0.164,0.222	0.127,0.222
Tmin'	0.033	

Correction method= MULTI-SCAN

Data completeness= 0.951 Theta(max)= 62.150

R(reflections)= 0.0619(22057) wR2(reflections)= 0.1520(28827)

S = 1.043 Npar= 1681

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 = 0.5735

PLAT029_ALERT_3_B	_diffrn_measured_fraction_theta_full	Low	0.95	
PLAT213_ALERT_2_B	Atom C1	has ADP max/min Ratio	4.20	prola
PLAT213_ALERT_2_B	Atom C2	has ADP max/min Ratio	4.20	prola
PLAT213_ALERT_2_B	Atom C3	has ADP max/min Ratio	4.20	prola
PLAT213_ALERT_2_B	Atom C4	has ADP max/min Ratio	4.20	prola
PLAT213_ALERT_2_B	Atom C5	has ADP max/min Ratio	4.20	prola
PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Cu3	-- P5 ..	13.75	su
PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Cu3	-- P7 ..	12.34	su
PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Cu3	-- P21 ..	10.68	su
PLAT232_ALERT_2_B	Hirshfeld Test Diff (M-X)	Fe10	-- P46 ..	13.86	su
PLAT242_ALERT_2_B	Check Low	Ueq as Compared to Neighbors for			Fe1B

● **Alert level C**

PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent		14	
PLAT213_ALERT_2_C	Atom C6	has ADP max/min Ratio	3.60	prola
PLAT213_ALERT_2_C	Atom C9	has ADP max/min Ratio	3.50	prola
PLAT213_ALERT_2_C	Atom C23	has ADP max/min Ratio	3.90	oblat
PLAT213_ALERT_2_C	Atom C52	has ADP max/min Ratio	3.40	prola
PLAT213_ALERT_2_C	Atom C53	has ADP max/min Ratio	3.20	prola
PLAT213_ALERT_2_C	Atom C63	has ADP max/min Ratio	3.60	oblat
PLAT213_ALERT_2_C	Atom C84	has ADP max/min Ratio	3.10	oblat
PLAT213_ALERT_2_C	Atom C88	has ADP max/min Ratio	3.10	oblat
PLAT220_ALERT_2_C	Large Non-Solvent	C	Ueq(max)/Ueq(min) ...	3.21	Ratio
PLAT222_ALERT_3_C	Large Non-Solvent	H	Ueq(max)/Ueq(min) ...	3.25	Ratio
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1	-- P6 ..	6.64	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Cu1	-- P11 ..	5.80	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe1	-- C4 ..	5.52	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe1	-- C5 ..	6.61	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe10	-- P47 ..	9.16	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe10	-- P48 ..	9.88	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe10	-- P49 ..	9.18	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe10	-- P50 ..	5.58	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe10	-- C91 ..	6.69	su
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X)	Fe10	-- C95 ..	5.21	su
PLAT250_ALERT_2_C	Large U3/U1 Ratio for Average U(i,j) Tensor		2.47	
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds (x 1000) Ang	...		12	
PLAT432_ALERT_2_C	Short Inter X...Y Contact	C14 .. C64 ..		3.20	Ang.
PLAT141_ALERT_4_C	su on a - Axis Small or Missing (x 100000)		10	Ang.
PLAT142_ALERT_4_C	su on b - Axis Small or Missing (x 100000)		20	Ang.
PLAT143_ALERT_4_C	su on c - Axis Small or Missing (x 100000)		20	Ang.
PLAT380_ALERT_4_C	Check Incorrectly? Oriented X(sp2)-Methyl Moiety			C16	
PLAT380_ALERT_4_C	Check Incorrectly? Oriented X(sp2)-Methyl Moiety			C18	

● **Alert level G**

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large.			220.40	
PLAT301_ALERT_3_G	Note Main Residue Disorder		8.00	Perc.
PLAT860_ALERT_3_G	Note: Number of Least-Squares Restraints		142	
PLAT302_ALERT_4_G	Note Anion/Solvent Disorder		50.00	Perc.
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.			P18	
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.			P19	
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.			P23	
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.			P24	
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.			P28	
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.			P29	
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.			P32	
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.			P33	
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.			P34	
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.			P37	
PLAT328_ALERT_4_G	Check for Possibly Missing H on sp3? Phosphorus.			P38	

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PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      P39
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      P42
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      P43
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      P44
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      >P46
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      >P47
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      >P48
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      >P49
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      >P50
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      <P46B
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      <P47B
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      <P48B
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      <P49B
PLAT328_ALERT_4_G Check for Possibly Missing H on sp3? Phosphorus.      <P50B
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure      !
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .....          9
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....      !
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 0 ALERT level A = In general: serious problem
12 ALERT level B = Potentially serious problem
29 ALERT level C = Check and explain
32 ALERT level G = General alerts; check
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 0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
32 ALERT type 2 Indicator that the structure model may be wrong or deficient
 7 ALERT type 3 Indicator that the structure quality may be low
33 ALERT type 4 Improvement, methodology, query or suggestion
 1 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 19/05/2009; check.def file version of 13/05/2009

