checkCIF/PLATON report

Structure factors have been supplied for datablock(s) comp_2, comp_4

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: comp_2

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Bond precision:   C-C = 0.0034 A          Wavelength=0.71073

Cell:             a=21.259(3)     b=24.250(4)         c=9.7919(15)
                  alpha=90        beta=93.137(2)      gamma=90
Temperature:      100 K
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	Calculated	Reported
Volume	5040.5(13)	5040.4(13)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C46 H56 Cl2 Cu2 Fe N4 P2 [+ solvent]	C46 H56 Cl2 Cu2 Fe N4 P2
Sum formula	C46 H56 Cl2 Cu2 Fe N4 P2 [+ solvent]	C46 H56 Cl2 Cu2 Fe N4 P2
Mr	980.74	980.71
Dx,g cm-3	1.292	1.292
Z	4	4
Mu (mm-1)	1.323	1.323
F000	2032.0	2032.0
F000'	2038.32	
h,k,lmax	29,33,13	28,32,13
Nref	6797	6693
Tmin,Tmax	0.760,0.890	0.612,0.815
Tmin'	0.760	

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Correction method= # Reported T Limits: Tmin=0.612 Tmax=0.815
AbsCorr = NUMERICAL

Data completeness= 0.985           Theta(max)= 29.145
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R(reflections)= 0.0421(5594) wR2(reflections)= 0.1003(6693)

S = 1.060 Npar= 262

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 C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.6 Ratio
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.1 Ratio

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Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 13.55 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 --Cl1 . 9.0 s.u.
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 466 A**3
PLAT793_ALERT_4_G Model has Chirality at P1 (Centro SPGR) R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1 (II) . 2.06 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 96 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 6 Info

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

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
2 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

Datablock: comp_4

Bond precision: C-C = 0.0044 A Wavelength=0.71073

Cell: a=22.086(6) b=23.767(7) c=9.834(3)
alpha=90 beta=92.224(4) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	5158(3)	5158(3)
Space group	C 2/c	C 1 2/c 1
Hall group	-C 2yc	-C 2yc
Moiety formula	C46 H56 Cu2 Fe I2 N4 P2 [+ solvent]	C46 H56 Cu2 Fe I2 N4 P2
Sum formula	C46 H56 Cu2 Fe I2 N4 P2 [+ solvent]	C46 H56 Cu2 Fe I2 N4 P2
Mr	1163.64	1163.61
Dx,g cm-3	1.498	1.498
Z	4	4
Mu (mm-1)	2.386	2.386
F000	2320.0	2320.0
F000'	2321.46	
h,k,lmax	30,32,13	29,32,13
Nref	6970	6857
Tmin,Tmax	0.775,0.830	0.354,0.760
Tmin'	0.515	

Correction method= # Reported T Limits: Tmin=0.354 Tmax=0.760
AbsCorr = NUMERICAL

Data completeness= 0.984 Theta(max)= 29.134

R(reflections)= 0.0403(5926) wR2(reflections)= 0.1135(6857)

S = 1.044 Npar= 262

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 C

PLAT220_ALERT_2_C	NonSolvent	Resd 1 C	Ueq(max)/Ueq(min) Range	4.6	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1	H	Uiso(max)/Uiso(min) Range	5.2	Ratio
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=		0.600	2	Report
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.85Ang From I1		2.16	eA-3
PLAT971_ALERT_2_C	Check Calcd Resid. Dens.	0.70Ang From Cu1		1.51	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.46Ang From I1		-1.62	eA-3
PLAT972_ALERT_2_C	Check Calcd Resid. Dens.	0.47Ang From I1		-1.53	eA-3

Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT	Unusually Large		29.78	Why ?
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	I1	--Cu1 .	20.0	s.u.
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X)	I1	--Cu1_a .	22.5	s.u.
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure			464	A**3

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PLAT793_ALERT_4_G Model has Chirality at P1          (Centro SPGR)          S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (II)      .       2.05 Info
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE  Suppressed          ! Info
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        103 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          2 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          8 Info
```

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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

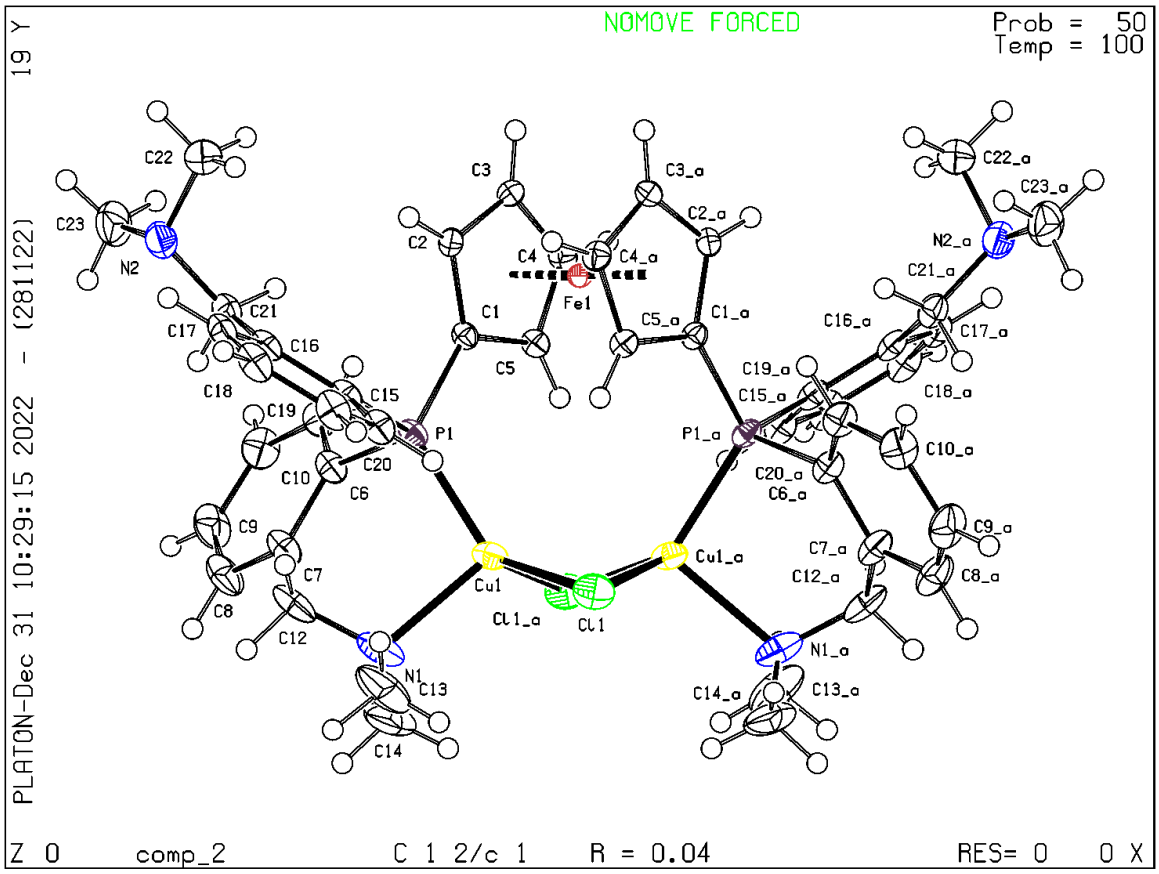
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, 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 28/11/2022; check.def file version of 28/11/2022

Datablock comp_2 - ellipsoid plot



Datablock comp_4 - ellipsoid plot