

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SK240_130K

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: SK240_130K

Bond precision:	C-C = 0.0041 A	Wavelength=1.34143
Cell:	a=19.3693(2)	b=20.3282(2) c=23.2111(2)
	alpha=90	beta=90 gamma=90
Temperature:	130 K	
	Calculated	Reported
Volume	9139.21(15)	9139.21(15)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C54 H44 Cu N2 O P2, F6 P	C54 H44 Cu1 F6 N2 O1 P3
Sum formula	C54 H44 Cu F6 N2 O P3	C54 H44 Cu1 F6 N2 O1 P3
Mr	1007.37	1007.41
Dx,g cm-3	1.464	1.464
Z	8	8
Mu (mm-1)	3.604	3.604
F000	4144.0	4144.0
F000'	4136.74	
h,k,lmax	24,25,29	24,25,28
Nref	9348	9298
Tmin,Tmax	0.395,0.486	0.882,0.951
Tmin'	0.295	

Correction method= # Reported T Limits: Tmin=0.882 Tmax=0.951
AbsCorr = INTEGRATION

Data completeness= 0.995 Theta(max)= 56.969

R(reflections)= 0.0563(8499) wR2(reflections)= 0.0502(9287)

S = 1.000 Npar= 604

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

```
PLAT413_ALERT_2_C Short Inter XH3 .. XHn      H401      ..H502      .      2.04 Ang.
                                     1-x,1-y,-z =      2_665 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=      0.600      11 Report
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) .      2 Check
PLAT939_ALERT_3_C Large Value of Not (SHELXL) Weight Optimized S .      16.07 Check
```

● Alert level G

```
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
                    not performed for this radiation type.
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ      Please Check
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing .....      0.00020 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing .....      0.00020 Ang.
PLAT244_ALERT_4_G Low      'Solvent' Ueq as Compared to Neighbors of      P3 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....      C50 Check
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found      Please Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=      0.600      50 Note
PLAT929_ALERT_5_G No Weight Pars,Obs and Calc R1,wR2,S not Checked      ! Info
PLAT984_ALERT_1_G The Cu-f'=-      -2.799 Deviates from the B&C-Value      -2.797 Ch
```

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **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
- 3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 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
5 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check
-

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT413_SK240_130K
;
PROBLEM: Short Inter XH3 .. XHn      H401      ..H502      .      2.04 Ang.
RESPONSE: ...
;
_vrf_PLAT911_SK240_130K
;
PROBLEM: Missing FCF Refl Between Thmin & STh/L=      0.600      11 Report
RESPONSE: ...
;
_vrf_PLAT918_SK240_130K
;
PROBLEM: Reflection(s) with I(obs) much Smaller I(calc) .      2 Check
RESPONSE: ...
;
_vrf_PLAT939_SK240_130K
;
PROBLEM: Large Value of Not (SHELXL) Weight Optimized S .      16.07 Check
RESPONSE: ...
;
# end Validation Reply Form
```

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.

