

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) SK245_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: SK245_130K

Bond precision: C-C = 0.0075 A

Wavelength=1.34143

Cell: a=11.7667(3) b=12.4566(3) c=16.3117(4)
 alpha=105.010(2) beta=93.514(2) gamma=108.465(2)
Temperature: 130 K

	Calculated	Reported
Volume	2163.43(10)	2163.43(10)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C51 H40 Cu N2 O P2, F6 P	C51 H40 Cu1 F6 N2 O1 P3
Sum formula	C51 H40 Cu F6 N2 O P3	C51 H40 Cu1 F6 N2 O1 P3
Mr	967.31	967.35
Dx,g cm-3	1.485	1.485
Z	2	2
Mu (mm-1)	3.790	3.790
F000	992.0	992.0
F000'	990.11	
h,k,lmax	14,15,20	14,15,20
Nref	8920	8709
Tmin,Tmax	0.524,0.685	0.200,0.897
Tmin'	0.384	

Correction method= # Reported T Limits: Tmin=0.200 Tmax=0.897
AbsCorr = MULTI-SCAN

Data completeness= 0.976

Theta(max)= 57.185

R(reflections)= 0.0957(7415)

wR2(reflections)= 0.0738(8691)

S = 0.893

Npar= 577

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

PLAT230_ALERT_2_C	Hirshfeld Test Diff for	C30	--C32	.	6.4 s.u.
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including		P3	0.082	Check
PLAT341_ALERT_3_C	Low Bond Precision on	C-C Bonds	0.00751	Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		47	Report

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
PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)	0.002 Degree
PLAT232_ALERT_2_G	Hirshfeld Test Diff (M-X) Cul --N1	9.5 s.u.
PLAT244_ALERT_4_G	Low 'Solvent' Ueq as Compared to Neighbors of	P3 Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C54 Check
PLAT790_ALERT_4_G	Centre of Gravity not Within Unit Cell: Resd. # F6 P	2 Note
PLAT808_ALERT_5_G	No Parseable SHELXL Style Weighting Scheme Found	Please Check
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	181 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	2 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
13 **ALERT level G** = General information/check it is not something unexpected
- 4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
4 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_PLAT230_SK245_130K
;
PROBLEM: Hirshfeld Test Diff for      C30      --C32      .      6.4 s.u.
RESPONSE: ...
;
_vrf_PLAT260_SK245_130K
;
PROBLEM: Large Average Ueq of Residue Including      P3      0.082 Check
RESPONSE: ...
;
_vrf_PLAT341_SK245_130K
;
PROBLEM: Low Bond Precision on  C-C Bonds .....      0.00751 Ang.
RESPONSE: ...
;
_vrf_PLAT911_SK245_130K
;
```

PROBLEM: Missing FCF Refl Between Thmin & STh/L= 0.600 47 Report
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.

PLATON version of 19/10/2018; check.def file version of 15/10/2018

