checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 20023

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: 20023

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Bond precision:  C-C = 0.0054 A          Wavelength=0.71073

Cell:            a=13.926(3)     b=13.293(3)         c=14.251(3)
                 alpha=90        beta=97.527(4)      gamma=90
Temperature:     150 K
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	Calculated	Reported
Volume	2615.4(10)	2615.3(11)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C26 H22 Cu N3 O S, F6 P	C26 H22 Cu N3 O S, F6 P
Sum formula	C26 H22 Cu F6 N3 O P S	C26 H22 Cu F6 N3 O P S
Mr	633.05	633.03
Dx,g cm-3	1.608	1.608
Z	4	4
Mu (mm-1)	1.045	1.045
F000	1284.0	1284.0
F000’	1286.84	
h,k,lmax	17,16,17	17,16,17
Nref	5129	5119
Tmin,Tmax	0.612,0.762	0.636,0.843
Tmin’	0.600	

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Correction method= # Reported T Limits: Tmin=0.636 Tmax=0.843
AbsCorr = EMPIRICAL

Data completeness= 0.998          Theta(max)= 25.997

R(reflections)= 0.0545( 3696)     wR2(reflections)= 0.1282( 5119)

S = 0.996                 Npar= 390
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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

PLAT232_ALERT_2_B Hirshfeld Test Diff (M-X) Cu1 --S1 . 20.1 s.u.

Author Response: The assignment of both Cu1 and S1 is correct and no residual disorder components are present.

Alert level C

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 7.121 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 8 Report

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 11 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 11 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 --N2 . 5.6 s.u.

Author Response: The assignment of both Cu1 and S1 is correct and no residual disorder components are present.

PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of P1 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 57% Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) . 2.27 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 153 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 3.9 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 1 Info

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

0 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
4 ALERT type 3 Indicator that the structure quality may be low
6 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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 18/09/2020; check.def file version of 20/08/2020

Datablock 20023 - ellipsoid plot