

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 9

Bond precision:	C-C = 0.0021 A	Wavelength=0.71073	
Cell:	a=14.0265(6)	b=7.5246(4)	c=14.4151(7)
	alpha=90	beta=90.172(4)	gamma=90
Temperature:	150 K		
	Calculated	Reported	
Volume	1521.42(13)	1521.42(13)	
Space group	P 21/n	P 1 21/n 1	
Hall group	-P 2yn	-P 2yn	
Moiety formula	C30 H34 Cu N4 O4, C3 H5 N	C30 H34 Cu N4 O4, C3 H5 N	
Sum formula	C33 H39 Cu N5 O4	C33 H39 Cu N5 O4	
Mr	633.24	633.23	
Dx,g cm-3	1.382	1.382	
Z	2	2	
Mu (mm-1)	0.764	0.764	
F000	666.0	666.0	
F000'	666.87		
h,k,lmax	19,10,20	19,10,20	
Nref	4586	3985	
Tmin,Tmax	0.548,0.737	0.692,1.000	
Tmin'	0.537		

Correction method= # Reported T Limits: Tmin=0.692 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.869 Theta(max)= 30.346

R(reflections)= 0.0315(3394) wR2(reflections)= 0.0854(3985)

S = 1.074 Npar= 219

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 G

PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size .. 0.80 mm
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 --N2 . 5.2 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of N3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C31 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C32 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C33 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H32B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33A Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33B Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H33C Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2) 4.50 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C110 ..C110 3.19 Ang.
2-x,2-y,1-z = 3_776 Check
PLAT789_ALERT_4_G Atoms with Negative _atom_site_disorder_group # 10 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2 Note
C3 H5 N
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) . 2.05 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
14 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 22/12/2019; check.def file version of 13/12/2019

