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: pabellondepicaite

Bond precision: O- N = 0.0200 A Wavelength=0.71075

Cell: a=7.2118(12) b=9.0983(15) c=11.128(3)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	730.2(3)	730.2(2)
Space group	P m m a	P m m a
Hall group	-P 2a 2a	-P 2a 2a
Moiety formula	2(C2 H5 Cl0.50 Cu N4.50 O1.50), 2(H2 O)	?
Sum formula	C4 H14 Cl Cu2 N9 O5	C4 H14 Cl Cu2 N9 O5
Mr	430.79	430.77
Dx,g cm-3	1.959	1.959
Z	2	2
Mu (mm-1)	3.131	3.131
F000	432.0	432.0
F000'	433.69	
h,k,lmax	7,9,11	7,9,11
Nref	560	555
Tmin,Tmax	0.672,0.954	0.294,1.000
Tmin'	0.659	

Correction method= # Reported T Limits: Tmin=0.294 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 22.464

R(reflections)= 0.0665(482) wR2(reflections)= 0.1601(555)

S = 1.098 Npar= 80

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 A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550
Calculated sin(theta_max)/wavelength = 0.5376

Alert level B

PLAT088_ALERT_3_B Poor Data / Parameter Ratio ..... 7.00 Note
PLAT780_ALERT_1_B Coordinates do not Form a Properly Connected Set Please Do !

Alert level C

PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cu2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N4 Check

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Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 8 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 8.81 Why ?
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 1 Note
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 4 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of O3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Hw1 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Hw2 Constrained at 0.5 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 5 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 25.10 Deg.
C -N1 -CU1 1_555 1_555 1_565 ..... # 44 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 25.10 Deg.
C -N1 -CU1 3_555 1_555 3_565 ..... # 48 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 33.32 Deg.
N2 -N2 -CU1 3_555 1_555 3_565 ..... # 55 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 25.40 Deg.
C -N2 -CU2 1_555 1_555 1_555 ..... # 57 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 24.90 Deg.
O1 -N4 -CU2 1_555 1_555 1_555 ..... # 71 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 24.90 Deg.
O1 -N4 -CU2 3_655 1_555 1_655 ..... # 73 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 30.60 Deg.
N1 -C -CU2 1_555 1_555 1_555 ..... # 79 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 30.40 Deg.
N2 -C -CU1 1_555 1_555 1_565 ..... # 80 Check
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF ... 28.90 Deg.
N2 -C -CU1 1_555 1_555 3_565 ..... # 83 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (I) . 1.29 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2 (I) . 1.38 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 8 Note

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PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  27 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 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
  16 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
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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 06/07/2023; check.def file version of 30/06/2023

Datablock pabellondepicaite - ellipsoid plot