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: 170423g

Bond precision: C-C = 0.0112 A Wavelength=0.71073

Cell: a=7.6974(7) b=12.6596(11) c=14.7907(12)
alpha=75.401(1) beta=79.650(2) gamma=81.089(2)
Temperature: 298 K

	Calculated	Reported
Volume	1362.9(2)	1362.9(2)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	2(C23 H21 Cl Cu2 N6 O2), 2(Cl), 2(H O0.50), 6(H2 O)	?
Sum formula	C46 H56 Cl4 Cu4 N12 O11	C46 H56 Cl4 Cu4 N12 O11
Mr	1349.03	1348.99
Dx,g cm-3	1.644	1.644
Z	1	1
Mu (mm-1)	1.804	1.804
F000	688.0	688.0
F000’	690.08	
h,k,lmax	9,15,17	9,15,17
Nref	4825	4737
Tmin,Tmax	0.730,0.777	0.579,0.786
Tmin’	0.536	

Correction method= # Reported T Limits: Tmin=0.579 Tmax=0.786
AbsCorr = MULTI-SCAN

Data completeness= 0.982 Theta(max)= 25.020

R(reflections)= 0.0670(3298) wR2(reflections)= 0.1911(4737)

S = 1.035 Npar= 361

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

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.01117 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 10 Report
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT093_ALERT_1_G No s.u.'s on H-positions, Refinement Reported as mixed Check
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu1 --Cl1_a . 6.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Cu2 --Cl1 . 11.3 s.u.
PLAT300_ALERT_4_G Atom Site Occupancy of O3 Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3C Constrained at 0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3D Constrained at 0.5 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 6% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 3 Note
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 22 Check
C1' -N1 -C1 1.555 1.555 1.555 28.80 Deg.
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle in CIF .... # 53 Check
C1 -C3 -C1' 1.555 1.555 1.555 28.40 Deg.
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2 (II) . 2.30 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 38 Note
PLAT899_ALERT_4_G SHELXL97 is Deprecated and Succeeded by SHELXL 2017 Note

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
8 ALERT type 4 Improvement, methodology, query or suggestion
4 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 09/11/2017; check.def file version of 08/11/2017

Datablock 170423g - ellipsoid plot