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: 1n

Bond precision: C-C = 0.0312 A Wavelength=0.71073

Cell: a=12.166(4) b=13.376(5) c=18.035(5)
alpha=68.76(2) beta=74.17(2) gamma=66.27(2)
Temperature: 100 K

	Calculated	Reported
Volume	2476.3(15)	2476.5(15)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C44 H33 Cu2 I2 N6 O2, 2(C H Cl3)	C44 H33 Cu2 I2 N6 O2, 2(C H Cl3)
Sum formula	C46 H35 Cl6 Cu2 I2 N6 O2	C46 H36 Cl6 Cu2 I2 N6 O2
Mr	1297.40	1298.39
Dx,g cm-3	1.740	1.741
Z	2	2
Mu (mm-1)	2.473	2.473
F000	1270.0	1272.0
F000’	1271.47	
h,k,lmax	14,16,21	14,16,21
Nref	9145	8187
Tmin,Tmax	0.427,0.431	0.425,0.745
Tmin’	0.395	

Correction method= # Reported T Limits: Tmin=0.425 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.895 Theta(max)= 25.438

R(reflections)= 0.1083(4960) wR2(reflections)= 0.3533(8187)

S = 1.228 Npar= 556

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

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.03119 Ang.

Author Response: The crystal was poorly diffracting at higher Bragg angles and this alert is comming due to poor data quality.

Alert level C

PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low . 0.961 Why?
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT082_ALERT_2_C High R1 Value ..... 0.11 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.35 Report
PLAT213_ALERT_2_C Atom C31 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom C34 has ADP max/min Ratio ..... 3.4 prolat
PLAT234_ALERT_4_C Large Hirshfeld Difference N2 --C6 . 0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference N6 --C36 . 0.18 Ang.
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C46 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C45 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cl4 0.183 Check
PLAT336_ALERT_2_C Long Bond Distance for ..... C45 -Cl5 1.900 Ang.

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: C46 H36 Cl6 Cu2 I2 N6 O2
Atom count from _chemical_formula_moiety:C46 H35 Cl6 Cu2 I2 N6 O2
FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:C46 H36 Cl6 Cu2 I2 N6 O2
Atom count from the _atom_site data: C46 H35 Cl6 Cu2 I2 N6 O2
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 2
From the CIF: _chemical_formula_sum C46 H36 Cl6 Cu2 I2 N6 O2
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	92.00	92.00	0.00
H	72.00	70.00	2.00
Cl	12.00	12.00	0.00
Cu	4.00	4.00	0.00
I	4.00	4.00	0.00
N	12.00	12.00	0.00
O	4.00	4.00	0.00

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.20 Report
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.02 Degree
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 4 Report
PLAT343_ALERT_2_G Unusual sp? Angle Range in Main Residue for C29 Check

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PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          6 Note
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON          8 Info
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed ..          ! Info
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         11 Note
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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
  12 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  15 ALERT level G = General information/check it is not something unexpected

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   9 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
   7 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 03/05/2019; check.def file version of 29/04/2019

Datablock 1n - ellipsoid plot