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: I

Bond precision: C-C = 0.0148 A Wavelength=0.71073

Cell: a=8.185(3) b=9.500(3) c=9.682(2)
alpha=69.01(3) beta=66.97(3) gamma=89.04(4)
Temperature: 293 K

	Calculated	Reported
Volume	640.2(4)	640.2(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C14 H6 Cl2 Cu2 N2 O8, Cu O6	C14 H6 Cl2 Cu3 N2 O14
Sum formula	C14 H6 Cl2 Cu3 N2 O14	C14 H6 Cl2 Cu3 N2 O14
Mr	687.76	687.73
Dx,g cm-3	1.784	1.784
Z	1	1
Mu (mm-1)	2.742	2.742
F000	337.0	337.0
F000’	338.42	
h,k,lmax	10,12,12	10,12,12
Nref	3149	2849
Tmin,Tmax	0.388,0.578	4.700,
Tmin’	0.244	

Correction method= # Reported T Limits: Tmin=4.700 Tmax=*****
AbsCorr = NUMERICAL

Data completeness= 0.905 Theta(max)= 28.208

R(reflections)= 0.0813(1626) wR2(reflections)= 0.2593(2849)

S = 1.015 Npar= 160

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

```
PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full value Low .      0.940 Why?
PLAT097_ALERT_2_B Large Reported Max.  (Positive) Residual Density       3.79 eA-3
PLAT430_ALERT_2_B Short Inter D...A Contact  O1       ..O5       .       2.68 Ang.
                                          1-x,1-y,-z  =      2_665 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O2       ..O5       .       2.73 Ang.
                                             x,y,z  =      1_555 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O3       ..O6       .       2.70 Ang.
                                          1-x,1-y,-z  =      2_665 Check
PLAT430_ALERT_2_B Short Inter D...A Contact  O4       ..O6       .       2.68 Ang.
                                           -x,-y,1-z  =      2_556 Check
```

Alert level C

```
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
           identifier.
           turquoise
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
DIFMX02_ALERT_1_C  The maximum difference density is > 0.1*ZMAX*0.75
           The relevant atom site should be identified.
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) .....................      0.26 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.55 Report
PLAT221_ALERT_2_C Solv./Anion  Resd 2  O   Ueq(max)/Ueq(min) Range        6.8 Ratio
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of        Cu2 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.2 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including       Cu2      0.102 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............    0.01483 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C1       - C2       .       1.53 Ang.
PLAT369_ALERT_2_C Long   C(sp2)-C(sp2) Bond  C6       - C7       .       1.53 Ang.
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of .         34 Ang**3
```

Alert level G

```
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.16 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported   _diffrn_ambient_temperature ..... (K)        293 Check
PLAT233_ALERT_4_G Hirshfeld (M-X Solvent)    Cu2      --O7       .        9.7 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.07 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2       (II)      .       2.01 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT883_ALERT_1_G No Info for _atom_sites_solution_primary .......     Please Do !
```

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

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  13 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
   3 ALERT type 4 Improvement, methodology, query or suggestion
   2 ALERT type 5 Informative message, check
```

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checkCIF publication errors

Alert level A

```
PUBL006_ALERT_1_A  _publ_requested_journal is missing
            e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
            Abstract of paper in English.
```

Alert level G

```
PUBL017_ALERT_1_G The _publ_section_references section is missing or
            empty.
```

```
   3 ALERT level A = Data missing that is essential or data in wrong format
   1 ALERT level G = General alerts. Data that may be required is missing
```

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
```

```
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 18/02/2019; check.def file version of 18/02/2019

Datablock I - ellipsoid plot