checkCIF/PLATON report

Structure factors have been supplied for datablock(s) I

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 = 0.0080 A Wavelength=1.54178

Cell: a=16.7185(6) b=22.0224(9) c=10.4938(4)
alpha=90 beta=90 gamma=90

Temperature: 200 K

	Calculated	Reported
Volume	3863.6(3)	3863.6(3)
Space group	P 21 21 2	P 21 21 2
Hall group	P 2 2ab	P 2 2ab
Moiety formula	C55 H90 Cl Cu N2 O28, C0.33 H0.33 Cl, 2(C0.67 H0.67 Cl2), 2(H2	C55 H90 Cl Cu N2 O28, 1.67(C H Cl2.99), 2(H2 O)
Sum formula	C56.67 H95.67 Cl5.99 Cu N2 O30	C56.67 H95.67 Cl5.98 Cu N2 O30
Mr	1560.81	1560.70
Dx,g cm-3	1.342	1.342
Z	2	2
Mu (mm-1)	2.974	2.973
F000	1640.9	1641.0
F000’	1646.31	
h,k,lmax	20,26,12	20,26,12
Nref	7094[3979]	7081
Tmin,Tmax	0.762,0.765	0.561,0.661
Tmin’	0.687	

Correction method= # Reported T Limits: Tmin=0.561 Tmax=0.661
AbsCorr = MULTI-SCAN

Data completeness= 1.78/1.00 Theta(max)= 68.307

R(reflections)= 0.0674(6305) wR2(reflections)= 0.2112(7081)

S = 1.039 Npar= 484

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

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT234_ALERT_4_C Large Hirshfeld Difference O6C --C9C . 0.16 Ang.
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cu1 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cl5 0.237 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cl2 0.162 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.008 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 10 Report
PLAT978_ALERT_2_C Number C-C Bonds with Positive Residual Density. 0 Info

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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: C56.67 H95.66999 Cl5.98 Cu1 N
Atom count from _chemical_formula_moiety:C56.67 H95.66999 Cl5.993300 C
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 11 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 6 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..... 2 Report
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ 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 0.16 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 7 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 1 Report
PLAT300_ALERT_4_G Atom Site Occupancy of C7B2 Constrained at 0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C7B Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7BD Constrained at 0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7BE Constrained at 0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7BF Constrained at 0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7BA Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7BB Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H7BC Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl5 Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl6 Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl7 Constrained at 0.3333 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C4 Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H4 Constrained at 0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2 Constrained at 0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3 Constrained at 0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl4 Constrained at 0.66 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3 Constrained at 0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3 Constrained at 0.6667 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 2% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O2B 109.7 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O6B 110.0 Degree
PLAT398_ALERT_2_G Deviating C-O-C Angle From 120 for O6C 109.0 Degree
PLAT432_ALERT_2_G Short Inter X...Y Contact Cl4 ..C9C 2.96 Ang.
1-x,1-y,1+z = 2_666 Check

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PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........         32 Note
PLAT780_ALERT_1_G Coordinates do not Form a Properly Connected Set     Please Do !
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (I)       .       0.81 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         31 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          3 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...         16 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
8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
45 **ALERT level G** = General information/check it is not something unexpected

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
12 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
27 ALERT type 4 Improvement, methodology, query or suggestion
3 ALERT type 5 Informative message, check

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checkCIF publication errors

Alert level A

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PUBL004_ALERT_1_A  The contact author’s name and address are missing,
           _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
           _publ_contact_author_phone are all missing.
           At least one of these should be present.
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.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
           Abstract of paper in English.
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7 **ALERT level A** = Data missing that is essential or data in wrong format
0 **ALERT level G** = General alerts. Data that may be required is missing

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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_PUBL004_GLOBAL
;
PROBLEM: The contact author’s name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
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 17/03/2019; check.def file version of 04/03/2019

Datablock I - ellipsoid plot