

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) 19zs_boo_d3_0m, 19zs_boo_d5_0ma, 19zs_boo_d8_dmpy4cu_0m, 20zs_boo_da4_CIPy3Cy_0m

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: 19zs_boo_d8_dmpy4cu_0m

Bond precision: C-C = 0.0088 Å Wavelength=0.71073

Cell: a=7.472(4) b=12.097(10) c=23.845(18)
 alpha=90 beta=94.822(13) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	2148(3)	2148(3)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C36 H40 Cu2 N4 O8 [+ solvent]	C18 H20 Cu N2 O4
Sum formula	C36 H40 Cu2 N4 O8 [+ solvent]	C19 H20 Cl2 Cu N2 O4
Mr	783.82	474.81
Dx, g cm ⁻³	1.212	1.469
Z	2	4
Mu (mm ⁻¹)	1.037	1.292
F000	812.0	972.0
F000'	813.58	
h,k,lmax	10,16,31	9,16,31
Nref	5418	5279
Tmin,Tmax	0.626,0.762	0.377,0.563
Tmin'	0.614	

Correction method= # Reported T Limits: Tmin=0.377 Tmax=0.563
AbsCorr = MULTI-SCAN

Data completeness= 0.974 Theta(max)= 28.475

R(reflections)= 0.0844(4606) wR2(reflections)= 0.2057(5279)

S = 1.224 Npar= 230

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	0.0088	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	6.397	Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	2.094	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	28	Report
PLAT934_ALERT_3_C	Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..	1	Check
PLAT975_ALERT_2_C	Check Calcd Resid. Dens. 0.97A From O1	0.61	eA-3
PLAT976_ALERT_2_C	Check Calcd Resid. Dens. 0.82A From O1	-0.74	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H16A	-0.53	eA-3
PLAT977_ALERT_2_C	Check Negative Difference Density on H16B	-0.37	eA-3



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: C19 H20 Cl2 Cu1 N2 O4
Atom count from _chemical_formula_moiety: C18 H20 Cu1 N2 O4

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: C19 H20 Cl2 Cu1 N2 O4
Atom count from the _atom_site data: C18 H20 Cu1 N2 O4

CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.

CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 4
From the CIF: _chemical_formula_sum C19 H20 Cl2 Cu N2 O4
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	76.00	72.00	4.00
H	80.00	80.00	0.00
Cl	8.00	0.00	8.00
Cu	4.00	4.00	0.00
N	8.00	8.00	0.00
O	16.00	16.00	0.00

PLAT012_ALERT_1_G	No _shelx_res_checksum Found in CIF	Please	Check
PLAT014_ALERT_1_G	No _shelx_fab_checksum Found in CIF	Please	Check
PLAT041_ALERT_1_G	Calc. and Reported SumFormula Strings Differ	Please	Check
PLAT042_ALERT_1_G	Calc. and Reported Moiety Formula Strings Differ	Please	Check
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	0.50	Check
PLAT051_ALERT_1_G	Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .	19.74	%
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	25.40	Why ?
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	254	A**3
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II) .	2.16	Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	2	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	108	Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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

9 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
5 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock: 19zs_boo_d3_0m

Bond precision: C-C = 0.0034 A Wavelength=0.71073
Cell: a=8.1473(6) b=22.5828(16) c=9.7106(7)
alpha=90 beta=105.399(2) gamma=90
Temperature: 100 K

	Calculated	Reported
Volume	1722.5(2)	1722.5(2)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C34 H36 Cu2 N4 O8	C34 H36 Cu2 N4 O8
Sum formula	C34 H36 Cu2 N4 O8	C34 H36 Cu2 N4 O8
Mr	755.77	755.75
Dx,g cm-3	1.457	1.457
Z	2	2
Mu (mm-1)	1.290	1.290
F000	780.0	780.0
F000'	781.57	
h,k,lmax	10,28,12	10,28,12
Nref	3495	3413
Tmin,Tmax	0.818,0.902	0.647,0.745
Tmin'	0.688	

Correction method= # Reported T Limits: Tmin=0.647 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 0.977 Theta(max)= 26.305

R(reflections)= 0.0280(2885) wR2(reflections)= 0.0721(3413)

S = 1.019 Npar= 220

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

PLAT220_ALERT_2_C NonSolvent	Resd 1 C	Ueq(max)/Ueq(min) Range	3.1 Ratio
PLAT911_ALERT_3_C Missing FCF Refl	Between Thmin & STh/L=	0.600	30 Report



Alert level G

PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II) .	2.16	Info
PLAT802_ALERT_4_G	CIF Input Record(s) with more than 80 Characters	2	Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	53	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.7	Low
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	5	Info

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0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
5 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: 19zs_boo_d5_0ma

Bond precision:	C-C = 0.0020 A	Wavelength=0.71073	
Cell:	a=11.1007(2)	b=20.4534(3)	c=9.8008(2)
	alpha=90	beta=101.247(1)	gamma=90
Temperature:	100 K		
	Calculated	Reported	
Volume	2182.51(7)	2182.51(7)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C44 H56 Cu2 N4 O8	C44 H56 Cu2 N4 O8	
Sum formula	C44 H56 Cu2 N4 O8	C44 H56 Cu2 N4 O8	
Mr	896.03	896.05	
Dx,g cm-3	1.363	1.363	
Z	2	2	
Mu (mm-1)	1.030	1.030	
F000	940.0	941.7	
F000'	941.62		
h,k,lmax	14,27,13	14,27,13	
Nref	5473	5471	
Tmin,Tmax	0.753,0.893	0.660,0.746	
Tmin'	0.727		

Correction method= # Reported T Limits: Tmin=0.660 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 28.390

R(reflections)= 0.0262(4787) wR2(reflections)= 0.0697(5471)

S = 1.033 Npar= 268

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

PLAT977_ALERT_2_C Check Negative Difference Density on H22C -0.31 eA-3



Alert level G

PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT073_ALERT_1_G H-atoms ref, but _hydrogen_treatment Reported as	constr Check
PLAT769_ALERT_4_G CIF Embedded explicitly supplied scattering data	Please Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1 (II) .	2.13 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters	2 Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600	6 Note
PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ...	3 Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.	15 Info
PLAT982_ALERT_1_G The Cu-f' = 0.3413 Deviates from IT-value =	0.3201 Check
PLAT983_ALERT_1_G The Cu-f" = 1.2895 Deviates from IT-Value =	1.2651 Check

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
10 **ALERT level G** = General information/check it is not something unexpected

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

Datablock: 20zs_boo_da4_CIPy3Cy_0m

Bond precision: C-C = 0.0025 A Wavelength=0.71073

Cell: a=8.1456(3) b=22.6010(7) c=9.7027(3)
 alpha=90 beta=105.571(1) gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	1720.70(10)	1720.70(10)
Space group	P 21/n	P 1 21/n 1
Hall group	-P 2yn	-P 2yn
Moiety formula	C32 H30 Cl2 Cu2 N4 O8	C32 H30 Cl2 Cu2 N4 O8
Sum formula	C32 H30 Cl2 Cu2 N4 O8	C32 H30 Cl2 Cu2 N4 O8
Mr	796.60	796.61
Dx,g cm-3	1.538	1.537
Z	2	2
Mu (mm-1)	1.446	1.446
F000	812.0	814.3
F000'	814.16	
h,k,lmax	10,29,12	10,28,12
Nref	3854	3843
Tmin,Tmax	0.655,0.793	0.556,0.746
Tmin'	0.614	

Correction method= # Reported T Limits: Tmin=0.556 Tmax=0.746
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 27.240

R(reflections)= 0.0252(3513) wR2(reflections)= 0.1084(3843)

S = 0.946 Npar= 219

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 G

PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT073_ALERT_1_G	H-atoms ref, but _hydrogen_treatment Reported as	constr Check
PLAT769_ALERT_4_G	CIF Embedded explicitly supplied scattering data	Please Note
PLAT794_ALERT_5_G	Tentative Bond Valency for Cu1 (II) .	2.14 Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	9 Note
PLAT933_ALERT_2_G	Number of OMIT Records in Embedded .res File ...	1 Note
PLAT960_ALERT_3_G	Number of Intensities with I < - 2*sig(I) ...	2 Check
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	8 Info
PLAT982_ALERT_1_G	The Cu-f'= 0.3413 Deviates from IT-value =	0.3201 Check
PLAT983_ALERT_1_G	The Cl-f"= 0.1603 Deviates from IT-Value =	0.1585 Check
PLAT983_ALERT_1_G	The Cu-f"= 1.2895 Deviates from IT-Value =	1.2651 Check

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

2 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

checkCIF publication errors

Alert level A

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.

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

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,
```

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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 22/03/2021; check.def file version of 19/03/2021







