

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: S- O = 0.0355 A Wavelength=1.79021

Cell: a=15.702 (2) b=15.702 (2) c=22.017 (5)
 alpha=90 beta=90 gamma=120

Temperature: 293 K

	Calculated	Reported
Volume	4701.1 (16)	4701.0 (2)
Space group	R 3	R 3
Hall group	R 3	R 3
Moiety formula	Cu11.07 Na12 O216 S54, *** (Na)	?
Sum formula	Cu11.07 Na68.55 O216 S54	Cu1.23 Na7.62 O24 S6
Mr	7466.70	830.77
Dx, g cm ⁻³	2.637	2.641
Z	1	9
Mu (mm ⁻¹)	15.115	15.115
F000	3667.1	1139.0
F000'	3698.01	
h, k, lmax	16, 16, 23	
Nref	2556 [1278]	
Tmin, Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.00/0.00 Theta (max)=

R(reflections)= 0.0521 (0) wR2(reflections)=
S = 7.700 Npar= 48 wR= 0.0770 (0)

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 A

GEOM001_ALERT_1_A _geom_bond_atom_site_label_1 is missing
Label identifying the atom site 1.
GEOM002_ALERT_1_A _geom_bond_atom_site_label_2 is missing
Label identifying the atom site 2.
GEOM003_ALERT_1_A _geom_bond_distance is missing
Distance between atom sites 1 and 2.
GEOM006_ALERT_1_A _geom_angle_atom_site_label_2 is missing
Label identifying the atom site 2.
GEOM007_ALERT_1_A _geom_angle_atom_site_label_3 is missing
Label identifying the atom site 3.
GEOM008_ALERT_1_A _geom_angle is missing
Angle between atom sites 1, 2 and 3.

Alert level B

PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	O3 Check
PLAT241_ALERT_2_B	High	'MainMol'	Ueq as Compared to Neighbors of	O18 Check
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	S2 Check
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	S3 Check
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	S4 Check
PLAT242_ALERT_2_B	Low	'MainMol'	Ueq as Compared to Neighbors of	S6 Check

- 6 **ALERT level A** = Most likely a serious problem - resolve or explain
6 **ALERT level B** = A potentially serious problem, consider carefully
9 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
28 **ALERT level G** = General information/check it is not something unexpected
18 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
16 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
12 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

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_GEOM001_I
;
PROBLEM: _geom_bond_atom_site_label_1 is missing RESPONSE: the selected interatomic distances are listed in
corresponding Table
;
_vrf_GEOM002_I
;
PROBLEM: _geom_bond_atom_site_label_2 is missing RESPONSE: the selected interatomic
distances are listed in corresponding Table
;
_vrf_GEOM003_I
;
PROBLEM: _geom_bond_distance is missing RESPONSE: the selected interatomic distances are
listed in corresponding Table
;
_vrf_GEOM006_I
;
PROBLEM: _geom_angle_atom_site_label_2 is missing RESPONSE: the selected interatomic
distances are listed in corresponding Table
;
_vrf_GEOM007_I
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;
PROBLEM: _geom_angle_atom_site_label_3 is missing RESPONSE: the selected interatomic
distances are listed in coresponding Table
;
_vrf_GEOM008_I
;
PROBLEM: _geom_angle is missing
RESPONSE: .the selected interatomic distances are listed in coresponding Table
;
_vrf_PLAT241_I
;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of O3 Check
RESPONSE: the powder was polluted by admixed petrovite and saranchinaite. Saranchinaite model
was not used during refinement, because of complexity of refinement with three phases. Thus, intensities of reflections are not properly
considered;
_vrf_PLAT242_I ;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of S2 Check
RESPONSE:the powder was polluted by admixed petrovite and saranchinaite. Saranchinaite model
was not used during refinement, because of complexity of refinement with three phases. Thus,
intensities of reflections are not properly considered
;

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# end Validation Reply Form
PLATON version of 18/05/2022; check.def file version of 17/05/2022

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