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: Cu- O = 0.0070 A Wavelength=0.39990

Cell: a=6.6791(6) b=15.5006(6) c=6.6811(6)
alpha=90 beta=90 gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	691.70(9)	691.70(10)
Space group	C m c m	C m c m
Hall group	-C 2c 2	-C -2x;-2yc
Moiety formula	Cu4 O8, 2(Cl), 3.6(O), 0.928(Sr)	?
Sum formula	Cl2 Cu4 O11.60 Sr0.93	Cu4 Cl2 O11.6 Sr0.928
Mr	592.01	592.00
Dx,g cm-3	2.842	2.842
Z	2	2
Mu (mm-1)	2.084	2.071
F000	556.1	556.0
F000'	558.60	
h,k,lmax	7,18,7	
Nref	345	
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.000 Theta(max)=

R(reflections)= 0.0796(0) wR2(reflections)=
wR= 0.0945(0)

S = 1.460 Npar= 47

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

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.

Alert level C

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.
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -C -2x; -2yc;-2
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of Cu1 Check
PLAT799_ALERT_4_C Numeric Label on Displacement Par. Record ..... ? Check

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.39990 Ang.
PLAT153_ALERT_1_G The s.u.'s on the Cell Axes are Equal ..(Note) 0.0006 Ang.
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3) 100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4) 100% Note
PLAT311_ALERT_2_G Isolated Disordered Oxygen Atom (No H's ?) ..... Ow Check
PLAT431_ALERT_2_G Short Inter HL..A Contact Cl1 ..Ow . 2.91 Ang.
3/2-x,1/2-y,-1/2+z = 10_654 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact Cl1 ..Ow . 2.91 Ang.
3/2-x,1/2-y,1-z = 13_656 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact Cl1 ..Ow . 2.91 Ang.
-1/2+x,-1/2+y,1/2-z = 14_445 Check
PLAT431_ALERT_2_G Short Inter HL..A Contact Cl1 ..Ow . 2.91 Ang.
-1/2+x,-1/2+y,z = 9_445 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..... 1 Note
PLAT984_ALERT_1_G The Cu-f'= 0.2377 Deviates from the B&C-Value 0.2366 Check
PLAT984_ALERT_1_G The Sr-f'= 0.2492 Deviates from the B&C-Value 0.2516 Check
PLAT985_ALERT_1_G The Cu-f"= 0.4448 Deviates from the B&C-Value 0.4425 Check

2 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
7 **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

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
6 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.

PLATON version of 13/07/2021; check.def file version of 13/07/2021

Datablock I - ellipsoid plot