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: Kalithallite

Bond precision: Tl-Cl = 0.0067 A Wavelength=1.79021

Cell: a=15.9333(5) b=15.9333(5) c=18.1008(7)
alpha=90 beta=90 gamma=90
Temperature: 297 K

	Calculated	Reported
Volume	4595.3(3)	4595.2(4)
Space group	I 4/m m m	I 4/m m m
Hall group	-I 4 2	-I 4 2
Moiety formula	2(Cl24 Tl4), Cl12 Tl1.32 Zn0.68, 2(Cl12 Tl2), 28(O), 40(K)	Cl6 K2.72 O1.714 Tl0.951 Zn0.049, 0.286(O)
Sum formula	Cl84 K40 O28 Tl13.32 Zn0.68	Cl6 K2.72 O2 Tl0.95 Zn0.05
Mr	7756.61	548.68
Dx,g cm-3	2.803	2.776
Z	1	14
Mu (mm-1)	60.449	55.290
F000	3511.3	0.0
F000'	3519.86	
h,k,lmax	16,16,18	
Nref	760	
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.000 Theta(max)=

R(reflections)= wR2(reflections)=
S = Npar=

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

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O1 Check

Author Response: These are the water molecules.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O2 Check

Author Response: These are the water molecules.

PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) ..... O3 Check

Author Response: These are the water molecules.

Alert level C

REFI015_ALERT_1_C _refine_ls_shift/su_max is missing
Maximum shift/s.u. ratio after final refinement cycle.
The following tests will not be performed
SHFSU_01
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 75.07 Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

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Alert level G

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:Cl6 K2.72 O2 Tl0.95 Zn.05
Atom count from the _atom_site data: Cl6 K2.857142 O2 Tl0.951428 Zn.0
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
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 14
From the CIF: _chemical_formula_sum Cl6 K2.72 O2 Tl0.95 Zn0.05
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Cl	84.00	84.00	0.00
K	38.08	40.00	-1.92
O	28.00	28.00	0.00
Tl	13.30	13.32	-0.02
Zn	0.70	0.68	0.02

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PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.071 Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka    1.79021 Ang.
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        71% Note
PLAT794_ALERT_5_G Tentative Bond Valency for Tl2       (III)     .       3.06 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Tl3       (III)     .       3.49 Info
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 ALERT level B = A potentially serious problem, consider carefully
   5 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

   8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 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
   3 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
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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 12/09/2022; check.def file version of 09/08/2022

Datablock Kalithallite - ellipsoid plot