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: 4789

Bond precision: = 0.0000 A Wavelength=0.71073

Cell: a=11.8405(3) b=12.7836(2) c=6.69165(16)
alpha=90 beta=112.425(3) gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	936.28(4)	936.29(4)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	As11.40 Cu0.08 Mg13.49 O48 P0.60, 3.216(Ca), 3.92(Na)	?
Sum formula	As11.40 Ca3.22 Cu0.08 Mg13.49 Na3.92 O48 P0.60	Al0.05 As2.85 Ca0.70 Cu0.02 Fe0.25 K0.01 Mg2.65 Mn0.05 Na1.24 O
Mr	2192.67	550.87
Dx,g cm-3	3.889	3.908
Z	1	4
Mu (mm-1)	10.975	11.326
F000	1040.8	1044.0
F000'	1043.36	
h,k,lmax	19,20,10	18,19,10
Nref	2041	1947
Tmin,Tmax	0.216,0.457	0.318,0.613
Tmin'	0.182	

Correction method= # Reported T Limits: Tmin=0.318 Tmax=0.613
AbsCorr = GAUSSIAN

Data completeness= 0.954 Theta(max)= 34.818

R(reflections)= 0.0227(1825) wR2(reflections)= 0.0465(1947)

S = 1.056 Npar= 101

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

PLAT075_ALERT_1_A Occupancy 1.018 Greater Than 1.0 for M1
PLAT075_ALERT_1_A Occupancy 1.177 Greater Than 1.0 for M2

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 10.81 Check
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by . 3.10 %
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check

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:Al.05 As2.85 Ca0.7 Cu.02 Fe0.25
Atom count from the _atom_site data: As2.85 Ca0.804 Cu.02 Mg3.372 Na0
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 Al0.05 As2.85 Ca0.70 Cu0.02 Fe0.25
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
Al	0.20	0.00	0.20
As	11.40	11.40	0.00
Ca	2.80	3.22	-0.42
Cu	0.08	0.08	0.00
Fe	1.00	0.00	1.00
K	0.04	0.00	0.04
Mg	10.60	13.49	-2.89
Mn	0.20	0.00	0.20
Na	4.96	3.92	1.04
O	48.00	48.00	0.00
P	0.60	0.60	0.00

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT017_ALERT_1_G Check Scattering Type Consistency of A1as CA
PLAT017_ALERT_1_G Check Scattering Type Consistency of A1’ as CU
PLAT017_ALERT_1_G Check Scattering Type Consistency of A2’as NA
PLAT017_ALERT_1_G Check Scattering Type Consistency of M1 as MG
PLAT017_ALERT_1_G Check Scattering Type Consistency of M2 as MG
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.25 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records 2 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K) 293 Check
PLAT200_ALERT_1_G Reported _diffrn_ambient_temperature ..... (K) 293 Check
PLAT300_ALERT_4_G Atom Site Occupancy of As1 Constrained at 0.95 Check
PLAT300_ALERT_4_G Atom Site Occupancy of As2 Constrained at 0.95 Check
PLAT300_ALERT_4_G Atom Site Occupancy of A1’ Constrained at 0.02 Check
PLAT300_ALERT_4_G Atom Site Occupancy of P1 Constrained at 0.05 Check
PLAT300_ALERT_4_G Atom Site Occupancy of P2 Constrained at 0.05 Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 20% 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
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels .........          5 Note
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
```

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

  17 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
  11 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 18/09/2020; check.def file version of 20/08/2020

Datablock 4789 - ellipsoid plot