checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

```
Bond precision:   P- O = 0.0020 A          Wavelength=0.71073

Cell:               a=13.6243(2)      b=10.3531(2)      c=6.3586(1)
                    alpha=90          beta=90           gamma=90
Temperature:        150 K
```

	Calculated	Reported
Volume	896.90(3)	896.90(3)
Space group	C m c m	C m c m
Hall group	-C 2c 2	-C 2c 2
Moiety formula	Cl4 Cu14.96 Na1.04 O36 P8, 8(Na)	Cl4 Cu14.96 Na1.04 O36 P8, 8(Na)
Sum formula	Cl4 Cu14.96 Na9.04 O36 P8	Cl Cu3.75 Na2.25 O9 P2
Mr	2124.10	531.39
Dx,g cm-3	3.933	3.935
Z	1	4
Mu (mm-1)	9.556	9.578
F000	1009.3	1010.0
F000'	1016.10	
h,k,lmax		19,14,8
Nref		733
Tmin,Tmax	0.301,0.516	0.706,1.000
Tmin'	0.194	

```
Correction method= # Reported T Limits: Tmin=0.706 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness=                 Theta(max)= 29.993

R(reflections)= 0.0170( 728)                    wR2(reflections)=
                                                0.0553( 733)
S = 0.992                  Npar= 57
```

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

```
PLAT220_ALERT_2_B NonSolvent   Resd 1 Cu   Ueq(max)/Ueq(min) Range        6.1 Ratio
```

Author Response: Thermal ellipsoids of the Cu are elongated because Cu(I)atoms occupy t

Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
              Calc: Cl Cu3.74 Na2.26 O9 P2
              Rep.: Cl Cu3.75 Na2.25 O9 P2
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.6 Note
PLAT975_ALERT_2_C Check Calcd Resid. Dens.  0.65Ang From O2      .       0.53 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:   Cl1 Cu3.75 Na2.25 O9 P2
            Atom count from _chemical_formula_moiety:Cl4 Cu14.96 Na9.04 O36 P8
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
           From the CIF: _cell_formula_units_Z    4
           From the CIF: _chemical_formula_sum  Cl Cu3.75 Na2.25 O9 P2
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           Cl         4.00      4.00    0.00
           Cu        15.00     14.96    0.04
           Na         9.00      9.04   -0.04
           O         36.00     36.00    0.00
           P          8.00      8.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...      0.250 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          1 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        17% Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.10 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2       (II)      .       2.05 Info
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          3 Info
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL     2019/3 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..       60.0 Degree
```

0 **ALERT level A** = Most likely a serious problem - resolve or explain

```
  1 ALERT level B = A potentially serious problem, consider carefully
  3 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

  6 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
  1 ALERT type 3 Indicator that the structure quality may be low
  4 ALERT type 4 Improvement, methodology, query or suggestion
  5 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 14/11/2023; check.def file version of 14/09/2023

Datablock shelx - ellipsoid plot