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: cokte

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

Cell:             a=5.611(1)     b=6.103(1)         c=23.808(5)
                  alpha=90       beta=95.18(3)      gamma=90
Temperature:      293 K
```

	Calculated	Reported
Volume	812.0(3)	811.9(3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	2(Cu4 H6 O14 S2), Co1.80 H24 Ni0.20 O12	Cu8.00 H12 O28 S4, Co1.8 H24 Ni0.2 O12
Sum formula	Co1.80 Cu8 H36 Ni0.20 O40 S4	H18 Co0.90 Cu4 Ni0.10 O20 S2
Mr	1430.74	715.33
Dx,g cm-3	2.926	2.926
Z	1	2
Mu (mm-1)	6.530	6.530
F000	706.2	706.0
F000’	710.33	
h,k,lmax	7,8,33	7,8,33
Nref	2371	2352
Tmin,Tmax	0.683,0.721	0.484,0.736
Tmin’	0.424	

```
Correction method= # Reported T Limits: Tmin=0.484 Tmax=0.736
AbsCorr = MULTI-SCAN

Data completeness= 0.992          Theta(max)= 30.040

R(reflections)= 0.0289( 1998)     wR2(reflections)= 0.0629( 2352)

S = 1.084                  Npar= 161
```

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

```
PLAT420_ALERT_2_B D-H Without Acceptor       O3       --H3       .     Please Check
```

Alert level C

```
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
PLAT199_ALERT_1_C Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_C Reported   _diffrn_ambient_temperature ..... (K)        293 Check
```

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:   H18 Co0.9 Cu4 Ni.1 O20 S2
            Atom count from _chemical_formula_moiety:H36 Co1.8 Cu8 Ni0.2 O40 S4
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         15 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found  in the CIF     Please Do !
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings  Differ     Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)...     Please Check
PLAT300_ALERT_4_G Atom Site Occupancy of Co         Constrained at        0.9 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Ni         Constrained at        0.1 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )        25% Note
PLAT794_ALERT_5_G Tentative Bond Valency for Cu1       (II)      .       2.00 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Cu2       (II)      .       2.12 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         12 Note
PLAT899_ALERT_4_G SHELXL97   is Deprecated and Succeeded by SHELXL       2018 Note
```

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

   7 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
   5 ALERT type 4 Improvement, methodology, query or suggestion
   4 ALERT type 5 Informative message, check
```

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_PLAT041_cokte
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...
;
_vrf_PLAT077_cokte
;
```

```
PROBLEM: Unitcell Contains Non-integer Number of Atoms ..     Please Check
RESPONSE: ...
;
_vrf_PLAT199_cokte
;
PROBLEM: Reported _cell_measurement_temperature ..... (K)        293 Check
RESPONSE: ...
;
_vrf_PLAT200_cokte
;
PROBLEM: Reported   _diffrn_ambient_temperature ..... (K)        293 Check
RESPONSE: ...
;
# end Validation Reply Form
```

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 22/12/2019; check.def file version of 13/12/2019

Datablock cokte - ellipsoid plot