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:   Ag-Ag = 0.0019 A         Wavelength=0.71073

Cell:               a=9.637(2)      b=12.946(3)          c=6.850(2)
                    alpha=90        beta=99.51(3)        gamma=90
Temperature:        297 K

                 Calculated                  Reported
Volume           842.9(4)                    842.9(4)
Space group      P c                         P 1 c 1
Hall group       P -2yc                      P -2yc
Moiety formula   Ag16 As7.81 S16 Sb0.19      ?
Sum formula      Ag16 As7.81 S16 Sb0.19      Ag2 As0.976 S2 Sb0.024
Mr               2846.90                     355.80
Dx,g cm-3        5.609                       5.608
Z                1                           8
Mu (mm-1)        17.809                      17.814
F000             1275.3                      1275.0
F000'            1263.59
h,k,lmax         12,17,9                     12,17,9
Nref             4095[ 2056]                 20050
Tmin,Tmax        0.448,0.779                 0.467,1.000
Tmin'            0.101

Correction method= # Reported T Limits: Tmin=0.467 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 9.75/4.90        Theta(max)= 28.070

R(reflections)= 0.0294( 18767)                wR2(reflections)=
                                              0.0793( 20050)
S = 1.605                  Npar= 267
```

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

PLAT881_ALERT_1_A No Datum for _diffrn_reflns_av_R_equivalents ... Please Do !

Alert level B

PLAT021_ALERT_4_B Ratio Unique / Expected Reflections too High ... 9.752
Unique Refl = 20050 / # Expected Refl = 2056

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: Ag2 As0.98 S2 Sb0.02
Rep.: Ag2 As0.976 S2 Sb0.024
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 7.70 Note
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Ag3 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Ag6 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Ag7 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of Ag8 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S2 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of S8 Check

Alert level G

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT005_ALERT_5_G No Embedded Refinement Details Found in the CIF Please Do !
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.125 Check
PLAT068_ALERT_1_G Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 20% Note
PLAT794_ALERT_5_G Tentative Bond Valency for Ag4 (I) . 1.07 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Ag5 (I) . 0.99 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT966_ALERT_5_G Note: Non-Standard (i.e. 2.0) OMIT Threshold of 3.0 Sig(I)

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

5 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
2 ALERT type 3 Indicator that the structure quality may be low
2 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.

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_PLAT881_I
;
PROBLEM: No Datum for _diffrn_reflns_av_R_equivalents ...     Please Do !
RESPONSE: ...Non-averaged data-set was used for the refinement, therefore no internal R
;            value is given.
_vrf_PLAT021_I
;
PROBLEM: Ratio Unique / Expected Reflections too High ...      9.752
RESPONSE: ... Non-averaged data-set was used for the refinement.
;
_vrf_PLAT041_I
;
PROBLEM: Calc. and Reported SumFormula    Strings  Differ     Please Check
RESPONSE: ...Differonly due to rounding errors.
;
_vrf_PLAT077_I
;
PROBLEM: Unitcell Contains Non-integer Number of Atoms ..     Please Check
RESPONSE: ...No it does not.
;
_vrf_PLAT090_I
```

;
PROBLEM: Poor Data / Parameter Ratio (Zmax > 18) ..... 7.70 Note
RESPONSE: ... The figure is somewhat smaller then ideal, but we discuss it accordingly.
;
_vrf_PLAT241_I
;
PROBLEM: High 'MainMol' Ueq as Compared to Neighbors of Ag3 Check
RESPONSE: ... Due to non-harmonic ADP.
;
_vrf_PLAT242_I
;
PROBLEM: Low 'MainMol' Ueq as Compared to Neighbors of S2 Check
RESPONSE: ... Somewhat lower than expected, but it is probably steric constraint.
;
end Validation Reply Form

PLATON version of 22/08/2024; check.def file version of 21/08/2024

Datablock I - ellipsoid plot