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: findsym-output

```
Bond precision:    = 0.0000 A                      Wavelength=0.71073

Cell:              a=6.81040       b=6.58878             c=5.60569
                   alpha=90        beta=125.2825         gamma=90
Temperature:       0 K

                   Calculated                  Reported
Volume             205.335                     0
Space group        C m                         C 1 m 1
Hall group         C -2y                       ?
Moiety formula     N3 Sb Zn3                   ?
Sum formula        N3 Sb Zn3                   ?
Mr                 359.96                      0.00
Dx,g cm-3          5.822                       0.000
Z                  2                           0
Mu (mm-1)          23.628                      0.000
F000               324.0                       0.0
F000'              324.65
h,k,lmax
Nref
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness=                  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 A

```
EXPT005_ALERT_1_A  _exptl_crystal_description is missing
           Crystal habit description.
           The following tests will not be performed.
           CRYSR_01
DIFF003_ALERT_1_A  _diffrn_measurement_device_type is missing
           Diffractometer make and type. Replaces _diffrn_measurement_type.
ATOM007_ALERT_1_A  _atom_site_aniso_label is missing
           Unique label identifying the atom site.
GEOM001_ALERT_1_A  _geom_bond_atom_site_label_1 is missing
           Label identifying the atom site 1.
GEOM002_ALERT_1_A  _geom_bond_atom_site_label_2 is missing
           Label identifying the atom site 2.
GEOM003_ALERT_1_A  _geom_bond_distance is missing
           Distance between atom sites 1 and 2.
GEOM006_ALERT_1_A  _geom_angle_atom_site_label_2 is missing
           Label identifying the atom site 2.
GEOM007_ALERT_1_A  _geom_angle_atom_site_label_3 is missing
           Label identifying the atom site 3.
PLAT029_ALERT_3_A _diffrn_measured_fraction_theta_full value Low .      0.000 Why?
PLAT043_ALERT_1_A Calculated and Reported Mol. Weight Differ by ..    359.96 Check
PLAT183_ALERT_1_A Missing _cell_measurement_reflns_used Value ....   Please Do !
PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value ......   Please Do !
PLAT185_ALERT_1_A Missing _cell_measurement_theta_max Value ......   Please Do !
PLAT197_ALERT_1_A Missing _cell_measurement_temperature Datum ....   Please Add
PLAT198_ALERT_1_A Missing _diffrn_ambient_temperature   Datum ....   Please Add
PLAT880_ALERT_1_A N0 datum for _diffrn_reflns_number .............   Please Do !
PLAT881_ALERT_1_A No Datum for _diffrn_reflns_av_R_equivalents ...   Please Do !
```

Alert level C

```
PLAT034_ALERT_1_C No Flack Parameter Given. Z > Si, NonCentro ....   Please Do !
PLAT141_ALERT_4_C s.u. on a - Axis Small or Missing ..............   0.00000 Ang.
PLAT142_ALERT_4_C s.u. on b - Axis Small or Missing ..............   0.00000 Ang.
PLAT143_ALERT_4_C s.u. on c - Axis Small or Missing ..............   0.00000 Ang.
PLAT145_ALERT_4_C s.u. on beta     Small or Missing ..............   0.0000 Degree
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .      ZN2 Check
PLAT161_ALERT_4_C Missing or Zero s.u. (esd) on x-coordinate for .      N1 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .      ZN2 Check
PLAT162_ALERT_4_C Missing or Zero s.u. (esd) on y-coordinate for .      N1 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .      ZN2 Check
PLAT163_ALERT_4_C Missing or Zero s.u. (esd) on z-coordinate for .      N1 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 ...     0.00 Check
PLAT128_ALERT_4_G Alternate Setting for Input Space Group  Cm            Im Note
PLAT794_ALERT_5_G Tentative Bond Valency for Sb1       (III)     .     3.32 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1       (II)      .     1.54 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Zn2       (II)      .     1.46 Info
PLAT808_ALERT_5_G No Parseable SHELXL Style Weighting Scheme Found  Please Check
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......   Please Do !
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .   Please Do !
PLAT980_ALERT_1_G No Anomalous Scattering Factors Found in CIF ...   Please Check
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   17 ALERT level A = Most likely a serious problem - resolve or explain
    0 ALERT level B = A potentially serious problem, consider carefully
   11 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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 11 ALERT level G = General information/check it is not something unexpected

 21 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  0 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
  6 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 17/03/2019; check.def file version of 04/03/2019