

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=8.90932 | b=8.90932 | c=8.90932 |
| | alpha=90 | beta=90 | gamma=90 |
| Temperature: | 0 K | | |
| | Calculated | Reported | |
| Volume | 707.186 | 0 | |
| Space group | F d -3 m | F 41/d -3 2 | |
| Hall group | -F 4vw 2vw | ? | |
| Moiety formula | N4 Sb2 Zn | ? | |
| Sum formula | N4 Sb2 Zn | ? | |
| Mr | 364.95 | 0.00 | |
| Dx,g cm-3 | 6.856 | 0.000 | |
| Z | 8 | 0 | |
| Mu (mm-1) | 21.695 | 0.000 | |
| F000 | 1280.0 | 0.0 | |
| F000' | 1273.28 | | |
| 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.

SYMMG01_ALERT_1_A Unrecognised _symmetry_space_group_name_H-M
From the CIF: _symmetry_Int_Tables_number 227
From the CIF: _symmetry_space_group_name_H-M F 41/d -3 2/m (origin
Int. Tables space group number for F 41/d -3 2/m (origin choice 2) is

SYMMG02_ALERT_1_A Supplied _symmetry_space_group_name_H-M not recognised
From the CIF: _symmetry_equiv_pos_as_xyz
x,y,z
x,-y+1/4,-z+1/4
-x+1/4,y,-z+1/4
-x+1/4,-y+1/4,z
y,z,x
y,-z+1/4,-x+1/4
-y+1/4,z,-x+1/4
-y+1/4,-z+1/4,x
z,x,y
z,-x+1/4,-y+1/4
-z+1/4,x,-y+1/4
-z+1/4,-x+1/4,y
-y,-x,-z
-y,x+1/4,z+1/4
y+1/4,-x,z+1/4
y+1/4,x+1/4,-z
-x,-z,-y
-x,z+1/4,y+1/4
x+1/4,-z,y+1/4
x+1/4,z+1/4,-y
-z,-y,-x
-z,y+1/4,x+1/4
z+1/4,-y,x+1/4
z+1/4,y+1/4,-x
-x,-y,-z
-x,y+1/4,z+1/4
x+1/4,-y,z+1/4
x+1/4,y+1/4,-z
-y,-z,-x
-y,z+1/4,x+1/4
y+1/4,-z,x+1/4
y+1/4,z+1/4,-x
-z,-x,-y
-z,x+1/4,y+1/4
z+1/4,-x,y+1/4
z+1/4,x+1/4,-y

y, x, z
 $y, -x+1/4, -z+1/4$
 $-y+1/4, x, -z+1/4$
 $-y+1/4, -x+1/4, z$
 x, z, y
 $x, -z+1/4, -y+1/4$
 $-x+1/4, z, -y+1/4$
 $-x+1/4, -z+1/4, y$
 z, y, x
 $z, -y+1/4, -x+1/4$
 $-z+1/4, y, -x+1/4$
 $-z+1/4, -y+1/4, x$
 $x, y+1/2, z+1/2$
 $x, -y+3/4, -z+3/4$
 $-x+1/4, y+1/2, -z+3/4$
 $-x+1/4, -y+3/4, z+1/2$
 $y, z+1/2, x+1/2$
 $y, -z+3/4, -x+3/4$
 $-y+1/4, z+1/2, -x+3/4$
 $-y+1/4, -z+3/4, x+1/2$
 $z, x+1/2, y+1/2$
 $z, -x+3/4, -y+3/4$
 $-z+1/4, x+1/2, -y+3/4$
 $-z+1/4, -x+3/4, y+1/2$
 $-y, -x+1/2, -z+1/2$
 $-y, x+3/4, z+3/4$
 $y+1/4, -x+1/2, z+3/4$
 $y+1/4, x+3/4, -z+1/2$
 $-x, -z+1/2, -y+1/2$
 $-x, z+3/4, y+3/4$
 $x+1/4, -z+1/2, y+3/4$
 $x+1/4, z+3/4, -y+1/2$
 $-z, -y+1/2, -x+1/2$
 $-z, y+3/4, x+3/4$
 $z+1/4, -y+1/2, x+3/4$
 $z+1/4, y+3/4, -x+1/2$
 $-x, -y+1/2, -z+1/2$
 $-x, y+3/4, z+3/4$
 $x+1/4, -y+1/2, z+3/4$
 $x+1/4, y+3/4, -z+1/2$
 $-y, -z+1/2, -x+1/2$
 $-y, z+3/4, x+3/4$
 $y+1/4, -z+1/2, x+3/4$
 $y+1/4, z+3/4, -x+1/2$
 $-z, -x+1/2, -y+1/2$
 $-z, x+3/4, y+3/4$
 $z+1/4, -x+1/2, y+3/4$
 $z+1/4, x+3/4, -y+1/2$
 $y, x+1/2, z+1/2$
 $y, -x+3/4, -z+3/4$
 $-y+1/4, x+1/2, -z+3/4$
 $-y+1/4, -x+3/4, z+1/2$
 $x, z+1/2, y+1/2$
 $x, -z+3/4, -y+3/4$
 $-x+1/4, z+1/2, -y+3/4$
 $-x+1/4, -z+3/4, y+1/2$
 $z, y+1/2, x+1/2$
 $z, -y+3/4, -x+3/4$
 $-z+1/4, y+1/2, -x+3/4$
 $-z+1/4, -y+3/4, x+1/2$
 $x+1/2, y, z+1/2$
 $x+1/2, -y+1/4, -z+3/4$

$-x+3/4, y, -z+3/4$
 $-x+3/4, -y+1/4, z+1/2$
 $y+1/2, z, x+1/2$
 $y+1/2, -z+1/4, -x+3/4$
 $-y+3/4, z, -x+3/4$
 $-y+3/4, -z+1/4, x+1/2$
 $z+1/2, x, y+1/2$
 $z+1/2, -x+1/4, -y+3/4$
 $-z+3/4, x, -y+3/4$
 $-z+3/4, -x+1/4, y+1/2$
 $-y+1/2, -x, -z+1/2$
 $-y+1/2, x+1/4, z+3/4$
 $y+3/4, -x, z+3/4$
 $y+3/4, x+1/4, -z+1/2$
 $-x+1/2, -z, -y+1/2$
 $-x+1/2, z+1/4, y+3/4$
 $x+3/4, -z, y+3/4$
 $x+3/4, z+1/4, -y+1/2$
 $-z+1/2, -y, -x+1/2$
 $-z+1/2, y+1/4, x+3/4$
 $z+3/4, -y, x+3/4$
 $z+3/4, y+1/4, -x+1/2$
 $-x+1/2, -y, -z+1/2$
 $-x+1/2, y+1/4, z+3/4$
 $x+3/4, -y, z+3/4$
 $x+3/4, y+1/4, -z+1/2$
 $-y+1/2, -z, -x+1/2$
 $-y+1/2, z+1/4, x+3/4$
 $y+3/4, -z, x+3/4$
 $y+3/4, z+1/4, -x+1/2$
 $-z+1/2, -x, -y+1/2$
 $-z+1/2, x+1/4, y+3/4$
 $z+3/4, -x, y+3/4$
 $z+3/4, x+1/4, -y+1/2$
 $y+1/2, x, z+1/2$
 $y+1/2, -x+1/4, -z+3/4$
 $-y+3/4, x, -z+3/4$
 $-y+3/4, -x+1/4, z+1/2$
 $x+1/2, z, y+1/2$
 $x+1/2, -z+1/4, -y+3/4$
 $-x+3/4, z, -y+3/4$
 $-x+3/4, -z+1/4, y+1/2$
 $z+1/2, y, x+1/2$
 $z+1/2, -y+1/4, -x+3/4$
 $-z+3/4, y, -x+3/4$
 $-z+3/4, -y+1/4, x+1/2$
 $x+1/2, y+1/2, z$
 $x+1/2, -y+3/4, -z+1/4$
 $-x+3/4, y+1/2, -z+1/4$
 $-x+3/4, -y+3/4, z$
 $y+1/2, z+1/2, x$
 $y+1/2, -z+3/4, -x+1/4$
 $-y+3/4, z+1/2, -x+1/4$
 $-y+3/4, -z+3/4, x$
 $z+1/2, x+1/2, y$
 $z+1/2, -x+3/4, -y+1/4$
 $-z+3/4, x+1/2, -y+1/4$
 $-z+3/4, -x+3/4, y$
 $-y+1/2, -x+1/2, -z$
 $-y+1/2, x+3/4, z+1/4$
 $y+3/4, -x+1/2, z+1/4$
 $y+3/4, x+3/4, -z$

```

-x+1/2,-z+1/2,-y
-x+1/2,z+3/4,y+1/4
x+3/4,-z+1/2,y+1/4
x+3/4,z+3/4,-y
-z+1/2,-y+1/2,-x
-z+1/2,y+3/4,x+1/4
z+3/4,-y+1/2,x+1/4
z+3/4,y+3/4,-x
-x+1/2,-y+1/2,-z
-x+1/2,y+3/4,z+1/4
x+3/4,-y+1/2,z+1/4
x+3/4,y+3/4,-z
-y+1/2,-z+1/2,-x
-y+1/2,z+3/4,x+1/4
y+3/4,-z+1/2,x+1/4
y+3/4,z+3/4,-x
-z+1/2,-x+1/2,-y
-z+1/2,x+3/4,y+1/4
z+3/4,-x+1/2,y+1/4
z+3/4,x+3/4,-y
y+1/2,x+1/2,z
y+1/2,-x+3/4,-z+1/4
-y+3/4,x+1/2,-z+1/4
-y+3/4,-x+3/4,z
x+1/2,z+1/2,y
x+1/2,-z+3/4,-y+1/4
-x+3/4,z+1/2,-y+1/4
-x+3/4,-z+3/4,y
z+1/2,y+1/2,x
z+1/2,-y+3/4,-x+1/4
-z+3/4,y+1/2,-x+1/4
-z+3/4,-y+3/4,x

```

These symops generate the Hall space group symbol `-f_4vw_2vw_3`
which is equivalent to the H-M space group symbol `f_d_-3_m`

| | | | | |
|-------------------|---------------------------------------|-----------------|---------|-------------|
| 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 .. | 364.95 | Check |
| PLAT129_ALERT_4_A | Unusual Space Group Specified | | F41/D-3 | Check |
| PLAT183_ALERT_1_A | Missing _cell_measurement_reflms_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_reflms_number | | | Please Do ! |
| PLAT881_ALERT_1_A | No Datum for _diffrn_reflms_av_R | equivalents ... | | Please Do ! |



Alert level C

| | | | |
|-------------------|---|---------|------|
| PLAT141_ALERT_4_C | s.u. on a - Axis Small or Missing | 0.00000 | Ang. |
|-------------------|---|---------|------|



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 |
| PLAT120_ALERT_1_G | Reported F41/d-3 Inconsistent with Explicit | Fd-3m | Check |
| PLAT794_ALERT_5_G | Tentative Bond Valency for Zn1 (II) | 1.54 | Info |
| PLAT808_ALERT_5_G | No Parseable SHELXL Style Weighting Scheme Found | | Please Check |
| PLAT882_ALERT_1_G | No Datum for _diffrn_reflms_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 |

20 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
1 **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

23 **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
2 **ALERT type 4** Improvement, methodology, query or suggestion
4 **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.

