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: Al- O = 0.0046 A Wavelength=0.71073

Cell: a=8.8448(4) b=13.3335(5) c=14.6837(8)
alpha=90 beta=115.753(4) gamma=90
Temperature: 873 K

	Calculated	Reported
Volume	1559.68(14)	1559.68(13)
Space group	I 2/a	I 2/a
Hall group	-I 2ya	-I 2ya
Moiety formula	Al16 As7.84 O64 Si8.16, 7.2(K), 8(Na0.10)	?
Sum formula	Al16 As7.84 K7.20 Na0.80 O64 Si8.16	Al2 As0.98 K0.90 Na0.10 O8 Si1.02 Zn0
Mr	2572.18	321.52
Dx,g cm-3	2.739	2.739
Z	1	8
Mu (mm-1)	5.153	5.153
F000	1238.6	1239.0
F000'	1242.65	
h,k,lmax	12,18,20	12,18,19
Nref	2159	1875
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.868 Theta(max)= 29.429

R(reflections)= 0.0584(1453) wR2(reflections)= 0.1214(1875)

S = 1.161 Npar= 118

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

PLAT196_ALERT_1_B No TEMP record and _measurement_temperature .NE. 293 Degree

Author Response: the temperature was 873 K

Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
             Calc: Al2 As0.98 K0.90 Na0.10 O8 Si1.02
             Rep.: Al2 As0.98 K0.90 Na0.10 O8 Si1.02 Zn0
PLAT052_ALERT_1_C Info on Absorption Correction Method   Not Given     Please Do !
PLAT053_ALERT_1_C Minimum Crystal Dimension Missing (or Error) ...     Please Check
PLAT054_ALERT_1_C Medium  Crystal Dimension Missing (or Error) ...     Please Check
PLAT055_ALERT_1_C Maximum Crystal Dimension Missing (or Error) ...     Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms ..     Please Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O1 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O2 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O3 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O4 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O5 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O6 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O7 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O8 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Al2 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     13.750 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.187 Check
```

Alert level G

```
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
            symmetry error - see SYMMG tests
           From the CIF: _cell_formula_units_Z    8
           From the CIF: _chemical_formula_sum  Al2 As0.98 K0.90 Na0.10 O8 Si1.02
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           Al        16.00     16.00    0.00
           As         7.84      7.84    0.00
           K          7.20      7.20    0.00
           Na         0.80      0.80    0.00
           O         64.00     64.00    0.00
           Si         8.16      8.16    0.00
           Zn         8.00      0.00    8.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          2 Info
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
PLAT128_ALERT_4_G Alternate Setting for Input Space Group  I2/a          C2/c Note
```

```
PLAT168_ALERT_4_G The CIF-Embedded .res File Contains EXYZ Records          3 Report
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records          3 Report
PLAT300_ALERT_4_G Atom Site Occupancy of As1        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of As2        Constrained at       0.48 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Si1        Constrained at        0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Si2        Constrained at       0.52 Check
PLAT300_ALERT_4_G Atom Site Occupancy of K1         Constrained at        0.9 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na1        Constrained at        0.1 Check
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd    1)        17% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    2)       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd    3)       100% Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT899_ALERT_4_G SHELXL2018 is Deprecated and Succeeded by SHELXL     2019/3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          4 Note
               1  1  0,   0  2  0,   0  1  1,   0  0  2,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        272 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.9 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ...........       2.73 Note
             Predicted wR2: Based on SigI**2  4.44 or SHELX Weight 10.80
```

---

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

11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
10 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
14 ALERT type 4 Improvement, methodology, query or suggestion
2 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 13/12/2023; check.def file version of 13/12/2023

Datablock shelx - ellipsoid plot