

## 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

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Bond precision:	Al- O = 0.0036 A	Wavelength=0.71073
Cell:	a=8.7896 (3)	b=13.3411 (5)      c=14.6916 (7)
	alpha=90	beta=115.824 (3)      gamma=90
Temperature:	473 K	
	Calculated	Reported
Volume	1550.74 (11)	1550.74 (11)
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	Al12 As0.98 K0.90 Na0.10 O8 Si1.02 Zn0
Mr	2572.18	321.52
Dx, g cm <sup>-3</sup>	2.754	2.754
Z	1	8
Mu (mm <sup>-1</sup> )	5.183	5.183
F000	1238.6	1239.0
F000'	1242.65	
h, k, lmax	12, 18, 20	11, 18, 19
Nref	2124	1866
Tmin, Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.879

Theta (max)= 29.343

R(reflections)= 0.0422 ( 1340)

wR2(reflections)=  
0.1057 ( 1866)

S = 0.954

Npar= 124

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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.

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#### Alert level B

PLAT196\_ALERT\_1\_B No TEMP record and \_measurement\_temperature .NE.

293 Degree

**Author Response: the temperature was 473 K**

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#### 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 01 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 02 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 03 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 04 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 06 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 07 Check

PLAT241\_ALERT\_2\_C High 'MainMol' Ueq as Compared to Neighbors of 08 Check

PLAT242\_ALERT\_2\_C Low 'MainMol' Ueq as Compared to Neighbors of A11 Check

PLAT906\_ALERT\_3\_C Large K Value in the Analysis of Variance ..... 5.283 Check

PLAT911\_ALERT\_3\_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report  
2 0 0, -2 2 2, -1 3 2, -5 11 10,

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#### 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). 1 1 0, 0 2 0, 0 1 1, 0 0 2,	4	Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	238	Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File 2 0 0, -2 2 2, -1 3 2, -5 11 10,	4	Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity .....	3.7	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 .....	1.91	Note
	Predicted wR2: Based on SigI**2 5.54 or SHELX Weight 11.46		

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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 1 **ALERT level B** = A potentially serious problem, consider carefully  
 16 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 25 **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

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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.

