

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 = 0.0025 A	Wavelength=0.71073	
Cell:	a=8.7661 (3)	b=13.3428 (4)	c=14.6781 (6)
	alpha=90	beta=115.893 (3)	gamma=90
Temperature:	300 K		
	Calculated	Reported	
Volume	1544.47 (10)	1544.46 (10)	
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 ⁻³	2.766	2.765	
Z	1	8	
Mu (mm ⁻¹)	5.204	5.204	
F000	1238.6	1239.0	
F000'	1242.65		
h, k, lmax	14, 21, 23	14, 20, 23	
Nref	3537	3288	
Tmin, Tmax			
Tmin'			

Correction method= Not given

Data completeness= 0.930

Theta (max)= 35.512

R(reflections)= 0.0508 (2366)

wR2(reflections)=
0.1083 (3288)

S = 1.042

Npar= 124

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 300 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 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 All Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 6.320 Check

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance 2.248 Check

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
0 2 2, -3 3 4,

PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.43Ang From O4 . -0.45 eA-3



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	226	Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File		3	Note
-3 3 4, -5 1 18, 0 2 2,			
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		2.23	Note
Predicted wR2: Based on SigI**2	4.85 or SHELX Weight	10.59	

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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
 14 **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
 7 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.

