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: O- B = 0.0106 A Wavelength=0.71073

Cell: a=8.414(5) b=10.173(6) c=15.905(10)
alpha=79.559(10) beta=78.675(9) gamma=70.912(11)
Temperature: 296 K

	Calculated	Reported
Volume	1251.4(13)	1251.3(13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	As2 B12 O24, B3 O6, 1.24(K), 0.76(Na)	?
Sum formula	As2 B15 K1.24 Na0.76 O30	As0.33 H0.50 B2.50 K0.21 Na0.13 O5
Mr	857.95	143.50
Dx,g cm-3	2.277	2.285
Z	2	12
Mu (mm-1)	3.021	3.022
F000	825.8	832.0
F000’	827.16	
h,k,lmax	11,14,22	11,14,22
Nref	7089	7031
Tmin,Tmax	0.930,0.970	0.885,1.000
Tmin’	0.913	

Correction method= # Reported T Limits: Tmin=0.885 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.992 Theta(max)= 29.711

R(reflections)= 0.0614(3436) wR2(reflections)= 0.1844(7031)

S = 0.954 Npar= 471

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

PLAT031_ALERT_4_B Refined Extinction Parameter Within Range ..... 2.000 Sigma

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Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
CRYSC01_ALERT_1_C The word below has not been recognised as a standard
identifier.
transparent
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by .. 3.05 Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT077_ALERT_4_C Unitcell Contains Non-integer Number of Atoms .. Please Check
PLAT213_ALERT_2_C Atom O18 has ADP max/min Ratio ..... 3.1 prolat
PLAT213_ALERT_2_C Atom O23 has ADP max/min Ratio ..... 3.4 prolat
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O17 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O23 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O24 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of O28 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of B14 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of B15 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.7 Note
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.3 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including K3 0.108 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 3.302 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 2 Report
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.86A From O30 -0.60 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.67A From O27 -0.53 eA-3

Alert level G

FORMU01_ALERT_2_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and the formula from the _atom_site* data.
Atom count from _chemical_formula_sum:H0.5 As0.33 B2.5 K0.21 Na0.13 O5
Atom count from the _atom_site data: As0.333333 B2.5 K0.206666 Na0.12
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G WARNING: H atoms missing from atom site list. Is this intentional?
From the CIF: _cell_formula_units_Z 12
From the CIF: _chemical_formula_sum As0.33 H0.50 B2.50 K0.21 Na0.13 O5
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
As	3.96	4.00	-0.04
H	6.00	0.00	6.00
B	30.00	30.00	0.00
K	2.52	2.48	0.04
Na	1.56	1.52	0.04
O	60.00	60.00	0.00

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT012_ALERT_1_G N.O.K. _shelx_res_checksum Found in CIF ..... Please Check
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.17 Check
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 1 Report

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PLAT300_ALERT_4_G Atom Site Occupancy of K2         Constrained at       0.58 Check
PLAT300_ALERT_4_G Atom Site Occupancy of K3         Constrained at       0.23 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Na2        Constrained at       0.19 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  3  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  4  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  5  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  6  )       100% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  7  )       100% Note
PLAT395_ALERT_2_G Deviating  X-O-Y    Angle From 120 for O13           130.7 Degree
PLAT397_ALERT_2_G Deviating  B-O-B    Angle From 120 for O4            130.2 Degree
PLAT397_ALERT_2_G Deviating  B-O-B    Angle From 120 for O11           131.5 Degree
PLAT397_ALERT_2_G Deviating  B-O-B    Angle From 120 for O21           133.3 Degree
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON          1 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).         3 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        52 Note
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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
 22 ALERT level C = Check. Ensure it is not caused by an omission or oversight
 23 ALERT level G = General information/check it is not something unexpected

 11 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 15 ALERT type 2 Indicator that the structure model may be wrong or deficient
  3 ALERT type 3 Indicator that the structure quality may be low
 15 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.

PLATON version of 07/08/2019; check.def file version of 30/07/2019

Datablock shelx - ellipsoid plot