checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ZnAs2H4O8

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: ZnAs2H4O8

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Bond precision:  As- O = 0.0044 A        Wavelength=0.71073

Cell:          a=4.9187(3)       b=5.2357(3)      c=12.8459(8)
               alpha=83.987(3)   beta=81.286(3)   gamma=80.117(3)
Temperature:   296 K
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	Calculated	Reported
Volume	321.09(3)	321.09(3)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	As2 O8 Zn	As2 O8 Zn
Sum formula	As2 O8 Zn	As2 H4 O8 Zn
Mr	343.23	347.24
Dx,g cm-3	3.550	3.592
Z	2	2
Mu (mm-1)	14.052	14.054
F000	320.0	328.0
F000’	321.02	
h,k,lmax	7,7,18	7,7,18
Nref	2049	2011
Tmin,Tmax	0.202,0.869	0.480,0.747
Tmin’	0.170	

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Correction method= # Reported T Limits: Tmin=0.480 Tmax=0.747
AbsCorr = MULTI-SCAN

Data completeness= 0.981          Theta(max)= 30.978

R(reflections)= 0.0380( 1600)     wR2(reflections)= 0.0994( 2011)

S = 1.032                 Npar= 100
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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.

Alert level B

PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by .. 4.01 Check

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)... Please Check
PLAT220_ALERT_2_C Non-Solvent Resd 1 O Ueq(max)/Ueq(min) Range 3.2 Ratio
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of As2 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 12 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 0.76A From As1 1.93 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.90A From O6 0.76 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.46A From O7 0.70 eA-3
PLAT975_ALERT_2_C Check Calcd Resid. Dens. 0.85A From O1 0.66 eA-3
PLAT976_ALERT_2_C Check Calcd Resid. Dens. 0.87A From O4 -0.60 eA-3

Alert level G

FORMU01_ALERT_1_G There is a discrepancy between the atom counts in the
_chemical_formula_sum and _chemical_formula_moiety. This is
usually due to the moiety formula being in the wrong format.
Atom count from _chemical_formula_sum: H4 As2 O8 Zn1
Atom count from _chemical_formula_moiety:As2 O8 Zn1
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:H4 As2 O8 Zn1
Atom count from the _atom_site data: As2 O8 Zn1
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 2
From the CIF: _chemical_formula_sum As2 H4 O8 Zn
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
As	4.00	4.00	0.00
H	8.00	0.00	8.00
O	16.00	16.00	0.00
Zn	2.00	2.00	0.00

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 2 Info
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note) 0.003 Degree
PLAT794_ALERT_5_G Tentative Bond Valency for Zn1 (II) . 1.98 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). 2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 25 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ... 2 Note
PLAT960_ALERT_3_G Number of Intensities with I < - 2*sig(I) ... 1 Check

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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
10 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
12 **ALERT level G** = General information/check it is not something unexpected

8 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 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
1 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 07/08/2019; check.def file version of 30/07/2019

Datablock ZnAs2H4O8 - ellipsoid plot