

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: evseevite

Bond precision: Mg- O = 0.0038 A Wavelength=1.79027

Cell: a=5.32235(12) b=14.1255(3) c=12.0047(3)
 alpha=90 beta=90 gamma=90

Temperature: 293 K

	Calculated	Reported
Volume	902.52(4)	902.53(4)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P -2xab;-2
Moiety formula	As4 F4 Mg4 O16, 8(Na)	?
Sum formula	As4 F4 Mg4 Na8 O16	As1 F1 Mg1 Na2 O4
Mr	912.84	228.20
Dx, g cm ⁻³	3.359	3.359
Z	2	8
Mu (mm ⁻¹)	19.543	20.042
F000	864.0	864.0
F000'	865.71	
h, k, lmax	5, 14, 12	
Nref	556	
Tmin, Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.000 Theta(max)=

R(reflections)= 0.0435(0)

wR2(reflections)=
wR= 0.0427(0)

S = 0.980

Npar= 77

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 C**

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -P -2xab;- Check
PLAT799_ALERT_4_C Numeric Label on Displacement Par. Record ? Check

● **Alert level G**

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.250 Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 1.79027 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints 10 Note
PLAT984_ALERT_1_G The As-f' = -0.6523 Deviates from the B&C-Value -0.6493 Check
PLAT985_ALERT_1_G The As-f" = 1.3109 Deviates from the B&C-Value 1.3143 Check

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

- 6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 - 0 ALERT type 2 Indicator that the structure model may be wrong or deficient
 - 1 ALERT type 3 Indicator that the structure quality may be low
 - 2 ALERT type 4 Improvement, methodology, query or suggestion
 - 1 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 28/11/2022; check.def file version of 28/11/2022

