

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: garpenbergite

Bond precision:	Sb- O = 0.0033 A	Wavelength=0.71073
Cell:	a=8.6790(9)	b=18.9057(19) c=6.1066(6)
	alpha=90	beta=90 gamma=90
Temperature:	293 K	
	Calculated	Reported
Volume	1001.99(18)	1001.99(18)
Space group	I m m a	I b m m
Hall group	-I 2b 2	?
	As3.56 Fe0.24 Mg5.92	
Moiety formula	Mn17.12 O48 Sb4 Si0.04	?
	Zn1.12	
	As3.56 Fe0.24 Mg5.92	As3.56 Fe0.24 Mg5.92
Sum formula	Mn17.12 O48 Sb4 Si0.04	Mn17.12 O48 Sb4 Si0.04
	Zn1.12	Zn1.12
Mr	2694.01	2694.01
Dx,g cm-3	4.465	4.465
Z	1	1
Mu (mm-1)	11.716	11.716
F000	1244.9	1250.0
F000'	1249.70	
h,k,lmax	14,31,10	14,31,10
Nref	1371	1317
Tmin,Tmax	0.536,0.626	0.445,0.561
Tmin'	0.520	

Correction method= # Reported T Limits: Tmin=0.445 Tmax=0.561
AbsCorr = MULTI-SCAN

Data completeness= 0.961 Theta(max)= 36.680

R(reflections)= 0.0367(957) wR2(reflections)= 0.1018(1317)

S = 0.990 Npar= 59

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

PLAT077_ALERT_4_C	Unitcell Contains Non-integer Number of Atoms ..	Please Check
PLAT199_ALERT_1_C	Reported _cell_measurement_temperature (K)	293 Check
PLAT200_ALERT_1_C	Reported _diffrn_ambient_temperature (K)	293 Check
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)	03 Check
PLAT313_ALERT_2_C	Oxygen with Three Covalent Bonds (rare)	04 Check



Alert level G

PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	3 Info
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please Check
PLAT300_ALERT_4_G	Atom Site Occupancy of As Constrained at	0.89 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Zn1 Constrained at	0.07 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Zn4 Constrained at	0.07 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mn1 Constrained at	0.71 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mn3 Constrained at	0.7 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mn4 Constrained at	0.71 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Fe Constrained at	0.06 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mn Constrained at	0.04 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Si Constrained at	0.01 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mg1 Constrained at	0.22 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mg3 Constrained at	0.3 Check
PLAT300_ALERT_4_G	Atom Site Occupancy of Mg4 Constrained at	0.22 Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	47% Note
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms	! Info
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL/	2018 Note

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 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
14 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

