

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: almagreraite

Bond precision:	= 0.0000 A	Wavelength=0.71075	
Cell:	a=5.7298 (4)	b=4.9715 (4)	c=9.3479 (7)
	alpha=90	beta=90	gamma=90
Temperature:	293 K		
	Calculated	Reported	
Volume	266.28 (3)	266.28 (3)	
Space group	P m n 21	P m n 21	
Hall group	P 2ac -2	P 2ac -2	
Moiety formula	Cu1.86 Mn5.72 O16 Zn1.80	?	
Sum formula	Cu1.86 Mn5.72 O16 Zn1.80	Cu0.94 Mn2.86 O8 Zn0.90	
Mr	806.16	403.37	
Dx, g cm ⁻³	5.027	5.031	
Z	1	2	
Mu (mm ⁻¹)	14.262	14.282	
F000	378.9	379.0	
F000'	382.15		
h,k,lmax	6,5,11	6,5,11	
Nref	515 [274]	522	
Tmin,Tmax	0.509,0.652	0.972,1.000	
Tmin'	0.116		

Correction method= # Reported T Limits: Tmin=0.972 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.91/1.01 Theta(max)= 25.009

R(reflections)= 0.0297 (423)	wR2(reflections)= 0.1103 (522)
S = 1.032	Npar= 75

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 A

PLAT090_ALERT_3_A Poor Data / Parameter Ratio (Zmax > 18) 3.65 Note

Alert level B

PLAT031_ALERT_4_B Refined Extinction Parameter Within Range of ... 2.143 Sigma

Alert level C

PLAT029_ALERT_3_C _diffn_measured_fraction_theta_full value Low . 0.974 Why?
PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: Cu1.86 Mn5.72 O16 Zn1.80
Rep.: Cu0.94 Mn2.86 O8 Zn0.90
PLAT077_ALERT_4_C Unit Cell Contains Non-integer Number of Atoms . Please Check
PLAT213_ALERT_2_C Atom O6 has ADP max/min Ratio 3.3 oblate

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: Cu0.94 Mn2.86 O8 Zn0.9
Atom count from the _atom_site data: Cu0.93 Mn2.86 O8 Zn0.9
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.500 Check
PLAT110_ALERT_2_G ADDSYM Detects Potential Lattice Translation ... ? Check
PLAT110_ALERT_2_G ADDSYM Detects Potential Lattice Translation ... ? Check
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem a/2 100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem 361 100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem 63 100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem c 100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem a/2 100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem 361 100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem 63 100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem m 100 %Fit
PLAT112_ALERT_2_G ADDSYM Detects New (Pseudo) Symm. Elem c 100 %Fit
PLAT116_ALERT_2_G ADDSYM Included (Pseudo) Lattice Translation ... Please Check
PLAT116_ALERT_2_G ADDSYM Included (Pseudo) Lattice Translation ... Please Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported _diffn_ambient_temperature (K) 293 Check
PLAT301_ALERT_3_G Main Residue Disorder (Resd 1) 44% Note
PLAT870_ALERT_4_G ALERTS Related to Twinning Effects Suppressed .. ! Info
PLAT883_ALERT_1_G Absent Datum for _atom_sites_solution_primary .. Please Do !
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 1 Note
2 5 0,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity 1.9 Low

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

5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
19 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 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.

