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: I

```
Bond precision:   C-C = 0.0250 A          Wavelength=0.69003

Cell:                a=7.844(4)       b=7.844(4)       c=6.985(5)
                     alpha=90         beta=90          gamma=120
Temperature:         293 K

                 Calculated                Reported
Volume           372.2(5)                  372.2(4)
Space group      P 6/m m m                 P 6/m m m
Hall group       -P 6 2                    -P 6;-2
Moiety formula   C12 Mn3 O17.94, 2(Cs)     ?
Sum formula      C12 Cs2 Mn3 O17.94        C12 Cs2 Mn3 O17.94
Mr               861.80                    861.80
Dx,g cm-3        3.845                     3.845
Z                1                         1
Mu (mm-1)        6.820                     2.942
F000             400.5                     401.0
F000'            400.97
h,k,lmax         10,10,9
Nref             224
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness= 0.000           Theta(max)=

                                                  wR2(reflections)=
R(reflections)= 0.0458( 0)                        wR= 0.0627( 0)
S = 1.890                 Npar= 55
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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

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Mn1 Check
PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.025 Ang.

Alert level C

CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -P 6;-2
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of O1 Check
PLAT799_ALERT_4_C Numeric Label on Displacement Par. Record ..... ? Check

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:C12 Cs2 Mn3 O17.94
Atom count from the _atom_site data: C12 Cs2 Mn3 O23.88
ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: Large difference may be due to a
symmetry error - see SYMMG tests
From the CIF: _cell_formula_units_Z 1
From the CIF: _chemical_formula_sum C12 Cs2 Mn3 O17.94
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	12.00	12.00	0.00
Cs	2.00	2.00	0.00
Mn	3.00	3.00	0.00
O	17.94	23.88	-5.94

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 1 Info
PLAT040_ALERT_1_G No H-atoms in this Carbon Containing Compound .. Please Check
PLAT092_ALERT_4_G Check: Wavelength Given is not Cu,Ga,Mo,Ag,In Ka 0.69003 Ang.
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 41% Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 2 Note
PLAT984_ALERT_1_G The Mn-f'= 0.3324 Deviates from the B&C-Value 0.3311 Check
PLAT985_ALERT_1_G The Cs-f"= 2.0362 Deviates from the B&C-Value 2.0231 Check
PLAT985_ALERT_1_G The Mn-f"= 0.6976 Deviates from the B&C-Value 0.6948 Check

0 **ALERT level A** = Most likely a serious problem - resolve or explain
2 **ALERT level B** = A potentially serious problem, consider carefully
4 **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

9 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

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  3 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
  2 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.

PLATON version of 13/07/2021; check.def file version of 13/07/2021

Datablock I - ellipsoid plot