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

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Bond precision:    C-C = 0.0170 A              Wavelength=0.69000

Cell:              a=7.4696(19)        b=7.4696(19)        c=5.847(4)
                   alpha=90            beta=90             gamma=120
Temperature:       293 K

                   Calculated                  Reported
Volume             282.5(2)                    282.5(2)
Space group        P 6/m m m                   P 6/m m m
Hall group         -P 6 2                      -P 6;-2
Moiety formula     C12 Mn5 O12                 ?
Sum formula        C12 Mn5 O12                 Mn5 C12 O12
Mr                 610.82                      610.80
Dx,g cm-3          3.590                       3.590
Z                  1                           1
Mu (mm-1)          5.060                       4.901
F000               293.0                       293.0
F000'              294.78
h,k,lmax           9,9,7
Nref               174
Tmin,Tmax
Tmin'

Correction method= Not given

Data completeness= 0.000            Theta(max)=

                                                    wR2(reflections)=
R(reflections)= 0.1298( 0)                          wR= 0.1549( 0)

S = 3.165                    Npar= 19
```

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
PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds ....   0.017 Ang.

🟡 Alert level C
CRYSC01_ALERT_1_C No recognised colour has been given for crystal colour.
PLAT041_ALERT_1_C Calc. and Reported SumFormula   Strings Differ   Please Check
PLAT082_ALERT_2_C High R1 Value ....   0.13 Report
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit   -P 6;-2

⚪ 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   2 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   0.69000 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact C1   ..C1   2.43 Ang.
                                            1-y,-1+x-y,z =   2_645 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C1   ..C1   2.43 Ang.
                                            2-x+y,1-x,z =   3_765 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact C1   ..C1   2.81 Ang.
                                            2-x,-y,z =   4_755 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1   (II)   .   2.00 Info
PLAT794_ALERT_5_G Tentative Bond Valency for Mn2   (II)   .   1.72 Info
PLAT984_ALERT_1_G The Mn-f'=   0.3324 Deviates from the B&C-Value   0.3311 Check
PLAT985_ALERT_1_G The Mn-f"=   0.6976 Deviates from the B&C-Value   0.6947 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
   4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
  11 **ALERT level G** = General information/check it is not something unexpected

   7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   4 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
   1 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.

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

Datablock I - ellipsoid plot

NOMOVE FORCED

Prob = 50
Temp = 293

56 Y

PLATON-Oct 25 03:03:58 2021 - (1307121)

Z -42   I   P 6/m m m   R = 0.13   RES= O 121 X