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: shelxl

Bond precision: Mg- O = 0.0030 A   Wavelength=0.71080

Cell: a=5.4215(11)   b=19.072(4)   c=5.3889(11)
               alpha=90   beta=110.21(3)   gamma=90
Temperature: 293 K

	Calculated	Reported
Volume	522.9(2)	522.89(18)
Space group	P 21	P 21
Hall group	P 2yb	P 2yb
Moiety formula	H10 Mg Mn2 O14 P2	?
Sum formula	H10 Mg Mn2 O14 P2	H10 Mg Mn2 O14 P2
Mr	430.21	426.08
Dx,g cm-3	2.732	2.706
Z	2	2
Mu (mm-1)	2.863	2.782
F000	428.0	424.0
F000'	430.09	
h,k,lmax	8,29,8	8,28,7
Nref	4157[2131]	3222
Tmin,Tmax	0.967,0.986	0.402,0.436
Tmin'	0.941	

Correction method= # Reported T Limits: Tmin=0.402 Tmax=0.436
AbsCorr = MULTI-SCAN

Data completeness= 1.51/0.78   Theta(max)= 33.650

R(reflections)= 0.0243(3204)   wR2(reflections)= 0.0618(3222)

S = 0.786   Npar= 208

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

```
TYPE033_ALERT_1_A  _cell_measurement_theta_min is not of type numb.
TYPE034_ALERT_1_A  _cell_measurement_theta_max is not of type numb.
PLAT184_ALERT_1_A Missing _cell_measurement_theta_min Value ......    Please Do !
PLAT185_ALERT_1_A Missing _cell_measurement_theta_max Value ......    Please Do !
PLAT430_ALERT_2_A Short Inter D...A Contact  O2        ..O8       .      2.49 Ang.
                                           1-x,-1/2+y,2-z  =      2_647 Check
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Alert level B

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PLAT420_ALERT_2_B D-H Bond Without Acceptor  Oh2       --H2       .     Please Check
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Alert level C

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ABSMU01_ALERT_1_C  The ratio of given/expected absorption coefficient lies
             outside the range 0.99 <> 1.01
         Calculated value of mu =     2.863
         Value of mu given       =     2.782
GOODF01_ALERT_2_C  The least squares goodness of fit parameter lies
         outside the range 0.80 <> 2.00
         Goodness of fit given =       0.786
RADNW01_ALERT_1_C  The radiation wavelength lies outside the expected range
         for the supplied radiation type. Expected range 0.71065-0.71075
         Wavelength given =     0.71080
PLAT043_ALERT_1_C Calculated and Reported Mol. Weight Differ by ..      4.13 Check
PLAT051_ALERT_1_C Mu(calc) and Mu(CIF) Ratio Differs from 1.0 by .      2.92 %
PLAT068_ALERT_1_C Reported F000 Differs from Calcd (or Missing)...    Please Check
PLAT199_ALERT_1_C Reported _cell_measurement_temperature ..... (K)      293 Check
PLAT200_ALERT_1_C Reported  _diffrn_ambient_temperature ..... (K)      293 Check
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       16 Note
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 !
PLAT033_ALERT_4_G Flack x Value Deviates > 3.0 * sigma from Zero .    0.072 Note
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...        2 Units
PLAT158_ALERT_4_G The Input Unitcell is NOT Standard/Reduced .....   Please Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........        6 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       15 Note
PLAT899_ALERT_4_G SHELXL97  is Deprecated and Succeeded by SHELXL/     2018 Note
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   5 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
   8 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

  12 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
   4 ALERT type 4 Improvement, methodology, query or suggestion
   2 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 22/03/2021; check.def file version of 19/03/2021