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: MgHDTMP_220C_publ

```
Bond precision:    C-C = 0.0153 A           Wavelength=1.54060

Cell:              a=23.4691(11)     b=8.6872(4)         c=9.6165(5)
                   alpha=90          beta=99.219(3)      gamma=90
Temperature:       493 K

                   Calculated                  Reported
Volume             1935.30(16)                 1935.3(2)
Space group        C 2/c                       C 2/c
Hall group         -C 2yc                      -C 2yn
Moiety formula     C10 Mg N2 O12 P4            ?
Sum formula        C10 Mg N2 O12 P4            C10 Mg N2 O12 P4
Mr                 488.31                      488.31
Dx,g cm-3          1.676                       0.000
Z                  4                           4
Mu (mm-1)          4.454                       0.000
F000               968.0                       0.0
F000'              976.66
h,k,lmax           19,7,8                      19,7,8
Nref               590                         588
Tmin,Tmax                                      1.000,1.000
Tmin'

Correction method= # Reported T Limits: Tmin=1.000 Tmax=1.000
AbsCorr = ?

Data completeness= 0.997         Theta(max)= 39.989

R(reflections)=                  wR2(reflections)=

S =                    Npar=
```

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

```
PLAT701_ALERT_1_A Bond    Calc   22.828(9), Rep    2.226(8), Dev..    2289.11 Sigma
            MG       -O1                 1.555-101.457 ........      #    2 Check
PLAT701_ALERT_1_A Bond    Calc   24.851(10), Rep   2.047(7), Dev..    2280.40 Sigma
            MG       -O4                 1.555-101.456 ........      #    4 Check
PLAT701_ALERT_1_A Bond    Calc   25.304(9), Rep    2.187(9), Dev..    2568.56 Sigma
            MG       -O5                 1.555-101.456 ........      #    6 Check
PLAT701_ALERT_1_A Bond    Calc   26.177(9), Rep    1.573(6), Dev..    2733.78 Sigma
            P1       -O2                 1.555-101.455 ........      #    8 Check
PLAT701_ALERT_1_A Bond    Calc   25.489(11), Rep   1.507(6), Dev..    2180.18 Sigma
            P1       -O3                 1.555-101.455 ........      #    9 Check
PLAT701_ALERT_1_A Bond    Calc   26.177(9), Rep    1.573(6), Dev..    2733.78 Sigma
            O2       -P1                 1.555-101.455 ........      #   17 Check
PLAT701_ALERT_1_A Bond    Calc   25.489(11), Rep   1.507(6), Dev..    2180.18 Sigma
            O3       -P1                 1.555-101.455 ........      #   18 Check
```

The checkcif program is not interpreting correctly the cif file creates by the GSAS program. All distances are right as it is shown by mercury/encifer programs

Alert level B

```
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ...............   0.01533 Ang.
```

Alert level C

```
PLAT127_ALERT_1_C Implicit Hall Symbol  Inconsistent with Explicit    -C 2yn
```

Alert level G

```
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   1.54060 Ang.
PLAT152_ALERT_1_G The Supplied and Calc. Volume s.u. Differ by ...      -4 Units
PLAT432_ALERT_2_G Short Inter X...Y Contact  O1       ..C1           2.69 Ang.
                                1/2-x,-1/2+y,3/2-z  =   102_546 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O2       ..C1           2.69 Ang.
                                  x,2-y,-1/2+z  =    -2_574 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O3       ..C1           2.81 Ang.
                                  x,2-y,-1/2+z  =    -2_574 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O4       ..C2           3.02 Ang.
                                1/2-x,1/2-y,-z  =  -101_555 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       31 Note
PLAT981_ALERT_1_G No non-zero f" Anomalous Scattering Values Found    Please Check
PLAT986_ALERT_1_G No non-zero f' Anomalous Scattering Values Found    Please Check
```

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  7 ALERT level A = Most likely a serious problem - resolve or explain
  1 ALERT level B = A potentially serious problem, consider carefully
  1 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

 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
  2 ALERT type 3 Indicator that the structure quality may be low
  1 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 14/07/2018; check.def file version of 05/06/2018