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: MgHDTMPH2O_publ

```
Bond precision:  C-C = 0.0163 A          Wavelength=1.54060

Cell:         a=12.5277(3)       b=9.70219(18)     c=8.62226(16)
              alpha=91.9174(13)  beta=70.6216(14)  gamma=86.4849(17)
Temperature:  298 K
```

	Calculated	Reported
Volume	985.16(4)	985.16(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C10 N2 O12 P4, O	?
Sum formula	C10 N2 O13 P4	C10 Mg1 N2 O13 P4
Mr	480.00	504.31
Dx,g cm-3	1.618	0.000
Z	2	2
Mu (mm-1)	4.116	0.000
F000	476.0	0.0
F000'	480.11	
h,k,lmax	12,9,8	12,9,8
Nref	2045	2044
Tmin,Tmax		1.000,1.000
Tmin'		

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

Data completeness= 1.000          Theta(max)= 49.995

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 B

```
PLAT043_ALERT_1_B Calculated and Reported Mol. Weight Differ by ..      24.31 Check
PLAT306_ALERT_2_B Isolated Oxygen Atom (H-atoms Missing ?) .......        H2O Check
PLAT340_ALERT_3_B Low Bond Precision on  C-C Bonds ..............    0.01633 Ang.
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Mg atom was not taken into account by the program in the sum formula. H-atoms were not localised by powder diffraction

Alert level C

```
PLAT041_ALERT_1_C Calc. and Reported SumFormula    Strings  Differ     Please Check
PLAT074_ALERT_1_C Occupancy Parameter = 0.0 for ..................        MG1 Check
PLAT074_ALERT_1_C Occupancy Parameter = 0.0 for ..................        MG2 Check
PLAT155_ALERT_4_C The Triclinic Unitcell is NOT Reduced ..........     Please Do !
```

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:C10 Mg1 N2 O13 P4
            Atom count from the _atom_site data:  C10 N2 O13 P4
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    2
           From the CIF: _chemical_formula_sum  C10 Mg1 N2 O13 P4
           TEST: Compare cell contents of formula and atom_site data

           atom    Z*formula  cif sites diff
           Mg         2.00      0.00    2.00
           P          8.00      8.00    0.00
           O         26.00     26.00    0.00
           C         20.00     20.00    0.00
           N          4.00      4.00    0.00
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 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.
PLAT300_ALERT_4_G Atom Site Occupancy of Mg1        Constrained at        0.0 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Mg2        Constrained at        0.0 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels ..........          1 Note
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............         64 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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   0 ALERT level A = Most likely a serious problem - resolve or explain
   3 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
   2 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
   5 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

Datablock MgHDTMPH2O_publ - ellipsoid plot