checkCIF/PLATON report

Structure factors have been supplied for datablock(s) shelx

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: shelx

```
Bond precision:  C-C = 0.0091 A          Wavelength=0.71073

Cell:           a=16.3632(19)    b=9.9059(11)      c=17.6686(18)
                alpha=90         beta=91.271(4)    gamma=90
Temperature:    150 K

                Calculated                Reported
Volume          2863.2(5)                 2863.2(5)
Space group     P 21/c                    P 21/c
Hall group      -P 2ybc                   -P 2ybc
Moiety formula  C26 H34 B2 Fe O6 W2       C26 H34 B2 Fe O6 W2
Sum formula     C26 H34 B2 Fe O6 W2       C26 H34 B2 Fe O6 W2
Mr              887.68                    887.70
Dx,g cm-3       2.059                     2.059
Z               4                         4
Mu (mm-1)       8.552                     8.552
F000            1688.0                    1688.0
F000'           1683.68
h,k,lmax        21,12,22                  21,12,22
Nref            6580                      6549
Tmin,Tmax       0.039,0.599               0.273,0.574
Tmin'           0.018

Correction method= # Reported T Limits: Tmin=0.273 Tmax=0.574
AbsCorr = MULTI-SCAN

Data completeness= 0.995          Theta(max)= 27.502

R(reflections)= 0.0359( 5763)     wR2(reflections)= 0.1025( 6549)

S = 1.040                  Npar= 357
```

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

```
PLAT972_ALERT_2_B Check Calcd Resid. Dens.  0.78A   From W1             -2.53 eA-3
```

Author Response: The electron density is found near the heavy atom Tungsten, which probably due to absorption error

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Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
            a literature citation. This should be contained in the
            _exptl_absorpt_process_details field.
            Absorption correction given as multi-scan
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0091 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         11 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.42A   From W1              1.78 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.02A   From W1              1.78 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.72A   From W2             -2.25 eA-3
```

Author Response: The electron density is found near the heavy atom Tungsten, which probably due to absorption error

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.80A   From W1             -2.22 eA-3
```

Author Response: The electron density is found near the heavy atom Tungsten, which probably due to absorption error

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.75A   From W2             -2.09 eA-3
```

Author Response: The electron density is found near the heavy atom Tungsten, which probably due to absorption error

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.75A   From W2             -2.02 eA-3
```

Author Response: The electron density is found near the heavy atom Tungsten, which probably due to absorption error

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.85A   From W1             -1.91 eA-3
```

Author Response: The electron density is found near the heavy atom Tungsten, which probably due to absorption error

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.84A   From W2             -1.69 eA-3
```

Author Response: The electron density is found near the heavy atom Tungsten, which probably due to absorption error

```
PLAT972_ALERT_2_C Check Calcd Resid. Dens.  0.94A   From C22            -1.58 eA-3
```

Author Response: The electron density is found near the heavy atom Tungsten, which probably due to absorption error

```
PLAT977_ALERT_2_C Check Negative Difference Density on H10A             -0.50 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H30C             -0.38 eA-3
```

Alert level G

```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      18.90 Why ?
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  W2       --B52      .        6.7 s.u.
PLAT303_ALERT_2_G Full Occupancy Atom H20       with # Connections       2.00 Check
PLAT303_ALERT_2_G Full Occupancy Atom H52B      with # Connections       2.00 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  O14      ..C30              3.01 Ang.
                                                  x,-1+y,z  =      1_545 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .       1.16 Ratio
PLAT779_ALERT_4_G Suspect or Irrelevant (Bond) Angle(s) in CIF . #        286 Check
              W2   -B52  -H52B    1.555   1.555   1.555             44.00 Deg.
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         21 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........        3.8 Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged     Please Check
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

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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
  14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  20 ALERT type 2 Indicator that the structure model may be wrong or deficient
   4 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   0 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 05/12/2020; check.def file version of 05/12/2020

Datablock shelx - ellipsoid plot