checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ABA2

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: ABA2

```
Bond precision:  C-C = 0.0221 A          Wavelength=0.71073

Cell:            a=18.1307(11)     b=34.026(2)     c=21.9349(13)
                 alpha=90          beta=90         gamma=90
Temperature:     299 K

                Calculated                Reported
Volume          13532.0(14)               13532.0(14)
Space group     A b a 2                   A b a 2
Hall group      A 2 -2ac                  A 2 -2ac
Moiety formula  C30 H45 B2 F6 O2 Ru3      ?
Sum formula     C30 H45 B2 F6 O2 Ru3      C30 H45 B2 F6 O2 Ru3
Mr              876.49                    876.49
Dx,g cm-3       1.721                     1.721
Z               16                        16
Mu (mm-1)       1.381                     1.381
F000            6992.0                    6992.0
F000'           6934.51
h,k,lmax        21,40,26                  21,40,26
Nref            11905[ 6129]              11883
Tmin,Tmax       0.725,0.813               0.650,0.860
Tmin'           0.701

Correction method= # Reported T Limits: Tmin=0.650 Tmax=0.860
AbsCorr = MULTI-SCAN

Data completeness= 1.94/1.00      Theta(max)= 25.000

R(reflections)= 0.0395( 10598)    wR2(reflections)= 0.0946( 11883)

S = 1.085                  Npar= 1005
```

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

```
PLAT214_ALERT_2_B Atom C2        (Anion/Solvent) ADP max/min Ratio        5.8 prolat
```

Author Response: This is due to the large thermal libration of cp* moieties which is expextd.

```
PLAT214_ALERT_2_B Atom B2        (Anion/Solvent) ADP max/min Ratio        5.8 oblate
```

Author Response: This is due to the large thermal libration of cp* moieties which is expextd.

```
PLAT220_ALERT_2_B NonSolvent   Resd 1  C   Ueq(max)/Ueq(min) Range        6.4 Ratio
```

Author Response: This is due to the large thermal libration of cp* moieties which is expextd.

```
PLAT342_ALERT_3_B Low Bond Precision on  C-C Bonds ...............    0.02207 Ang.
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Author Response: There are still disorders associated with cp* moiety might have affected the bond precision.

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PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min).         13 Note
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Author Response: Could be the unresolvable reflection during frame integration.

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PLAT934_ALERT_3_B Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          2 Check
```

Alert level C

```
STRVA01_ALERT_4_C           Flack test results are ambiguous.
           From the CIF: _refine_ls_abs_structure_Flack    0.480
           From the CIF: _refine_ls_abs_structure_Flack_su    0.080
PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ........       6.08 Note
PLAT213_ALERT_2_C Atom B3              has ADP max/min Ratio .....        3.1 oblate
PLAT214_ALERT_2_C Atom C30       (Anion/Solvent) ADP max/min Ratio        4.1 prolat
```

Author Response: This is due to the large thermal libration of cp* moieties which is expextd.

```
PLAT221_ALERT_2_C Solv./Anion  Resd 2  C   Ueq(max)/Ueq(min) Range        4.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference F10      --B4       .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference O4       --B4       .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C33'     --C38'     .       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C41      --C46      .       0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C42      --C47      .       0.24 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference F3       --B1       .       0.16 Ang.
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Ru5 Check
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PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         B3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Ru3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        C21 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         B1 Check
PLAT412_ALERT_2_C Short Intra XH3 .. XHn     H6C      ..H29C     .       1.82 Ang.
                                                      x,y,z  =      1_555 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.595          2 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF ....          4 Note
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Alert level G

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PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite         74 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...        104 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      86.34 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records         10 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records         15 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records         15 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records          1 Report
PLAT301_ALERT_3_G Main Residue  Disorder ..............(Resd  1  )        47% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )         9% Note
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C36' Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C37' Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C38' Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C39' Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....       C40' Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C46 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C47 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C48 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C49 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C50 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C6 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C7 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C8 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....         C9 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C10 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C16 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C17 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C18 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C19 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C20 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C26 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C27 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C28 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C29 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C30 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H39E     ..H48B     .       1.92 Ang.
                                                      x,y,z  =      1_555 Check
PLAT412_ALERT_2_G Short Intra XH3 .. XHn     H46B     ..H58B     .       2.06 Ang.
                                                      x,y,z  =      1_555 Check
PLAT811_ALERT_5_G No ADDSYM Analysis: Too Many Excluded Atoms ....          ! Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       1625 Note
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT909_ALERT_3_G Percentage of I>2sig(I) Data at Theta(Max) Still        78% Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File ...          6 Note
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
   6 ALERT level B = A potentially serious problem, consider carefully
  19 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  43 ALERT level G = General information/check it is not something unexpected
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  1 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
  9 ALERT type 3 Indicator that the structure quality may be low
 37 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 05/12/2020; check.def file version of 05/12/2020

Datablock ABA2 - ellipsoid plot