checkCIF/PLATON report

Structure factors have been supplied for datablock(s) cu420, cu652, moa537

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: moa537

Bond precision:  C-C = 0.0033 A  Wavelength=0.71073

Cell:  
\[
\begin{align*}
    a &= 7.6996(3) \\
    b &= 11.8327(5) \\
    c &= 12.8523(5) \\
    \alpha &= 83.018(3) \\
    \beta &= 77.340(3) \\
    \gamma &= 73.084(3)
\end{align*}
\]

Temperature:  150 K

| Calculated | Reported |
|------------|----------|
| 1090.94(8) | 1090.94(8) |

Space group  
P -1

Hall group  
-P 1

Moiety formula  
C22 H25 Cl F3 N O2 Ru

Sum formula  
C22 H25 Cl F3 N O2 Ru

Mr  
528.95

Dx, g cm\(^{-3}\)  
1.610

Z  
2

Mu (mm\(^{-1}\))  
0.885

F000  
536.0

F000'  
534.02

h,k,lmax  
10,16,18

Nref  
6502

Tmin,Tmax  
0.915,0.957

Correction method= # Reported T Limits: Tmin=0.746 Tmax=1.000

AbsCorr = MULTI-SCAN

Data completeness= 0.865  
Theta(max)= 30.262

R(reflections)= 0.0330( 4701)  
wR2(reflections)= 0.0599( 5622)

S = 0.997  
Npar= 276

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 C

**PLAT213_ALERT_2_C**  Atom F1A  has ADP max/min Ratio .....  3.2 prolat

**PLAT910_ALERT_3_C**  Missing # of FCF Reflection(s) Below Theta(Min).  5 Note

### Alert level G

**PLAT154_ALERT_1_G**  The s.u.’s on the Cell Angles are Equal ..(Note)  0.003 Degree

**PLAT912_ALERT_3_G**  Missing # of FCF Reflections Above STh/L= 0.600  795 Note

**PLAT941_ALERT_4_G**  Average HKL Measurement Multiplicity ...........  1.7 Low

**PLAT952_ALERT_5_G**  Calculated (ThMax) and CIF-Reported Lmax Differ  2 Units

**PLAT958_ALERT_1_G**  Calculated (ThMax) and Actual (FCF) Lmax Differ  2 Units

**PLAT978_ALERT_2_G**  Number C-C Bonds with Positive Residual Density.  7 Info

### ALERT level A = Most likely a serious problem - resolve or explain

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### ALERT level C = Check. Ensure it is not caused by an omission or oversight

### ALERT level G = General information/check it is not something unexpected

### ALERT type 1 CIF construction/syntax error, inconsistent or missing data

### ALERT type 2 Indicator that the structure model may be wrong or deficient

### ALERT type 3 Indicator that the structure quality may be low

### ALERT type 4 Improvement, methodology, query or suggestion

### ALERT type 5 Informative message, check

### Datablock: cu420

**Bond precision:**  \( C-C = 0.0109 \) Å  \( \text{Wavelength=1.54184} \)

**Cell:**
- \( a=11.9977(4) \) Å  \( b=16.2064(6) \) Å  \( c=16.7303(6) \) Å
- \( \alpha=90 \) °  \( \beta=100.767(3) \) °  \( \gamma=90 \) °

**Temperature:**  150 K

**Volume**
- Calculated: 3195.8(2) Å³
- Reported: 3195.8(2) Å³

**Space group**
- Calculated: \( P\ 2\ 1/n \)
- Reported: \( P\ 1\ 2\ 1/n\ 1 \)

**Hall group**
- Calculated: \( -P\ 2yn \)
- Reported: \( -P\ 2yn \)

**Moiety formula**
- Calculated: \( C_{28}\ H_{37}\ F_{3}\ N_{4}\ O_{2}\ P\ Ru,\ F_{6}\ P \)
- Reported: \( C_{28}\ H_{37}\ F_{3}\ N_{4}\ O_{2}\ P\ Ru,\ F_{6}\ P \)

**Sum formula**
- Calculated: \( C_{28}\ H_{37}\ F_{9}\ N_{4}\ O_{2}\ P_{2}\ Ru \)
- Reported: \( C_{28}\ H_{37}\ F_{9}\ N_{4}\ O_{2}\ P_{2}\ Ru \)

**Mr**
- Calculated: 795.63
- Reported: 795.62

**Dx,g cm\(^{-3}\)**
- Calculated: 1.654
- Reported: 1.654

**Z**
- Calculated: 4
- Reported: 4

**Mu (mm\(^{-1}\))**
- Calculated: 5.705
- Reported: 5.705

**F000**
- Calculated: 1616.0
- Reported: 1616.0

**F000’**
- Calculated: 1624.01

**h,k,lmax**
- Calculated: 14,19,20
- Reported: 14,19,20

**Nref**
- Calculated: 6078
- Reported: 6060

**Tmin,Tmax**
- Calculated: 0.789,0.843
- Reported: 0.286,1.000

**Tmin’**
- Calculated: 0.716

Correction method= # Reported T Limits: Tmin=0.286 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta(max)= 70.073
R(reflections)= 0.0640 (4779) wR2(reflections)= 0.1860 (6060)
S = 1.041 Npar= 418

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 | Test Name | Alert Type | Alert Level | Description |
|---------------|-----------|------------|-------------|-------------|
| PLAT213_ALERT_2_B | Atom C23 | has ADP max/min Ratio | 4.8 prol | ..... |
| PLAT220_ALERT_2_B | NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range | 8.4 Ratio | 0.19 Ang. |
| PLAT242_ALERT_2_B | Low ‘MainMol’ Ueq as Compared to Neighbors of C21 Check | |

| Alert level C | Test Name | Alert Type | Alert Level | Description |
|---------------|-----------|------------|-------------|-------------|
| PLAT213_ALERT_2_C | Atom C18 | has ADP max/min Ratio | 3.8 prol | ..... |
| PLAT222_ALERT_3_C | NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range | 8.9 Ratio | |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for C21 --C22 | 5.5 s.u. | |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C18 --C19 | 0.19 Ang. | |
| PLAT244_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of C1 Check | |
| PLAT250_ALERT_2_C | Large Average Ueq of Residue Including P34 | 0.109 Check | |
| PLAT342_ALERT_3_C | Low Bond Precision on C-C Bonds | 0.0109 Ang. | |
| PLAT860_ALERT_3_G | Number of Distance or Angle Restraints on AtSite | 3 Note | |
| PLAT242_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of C21 Check | |
| PLAT244_ALERT_4_G | Low ‘Solvent’ Ueq as Compared to Neighbors of P34 Check | |
| PLAT380_ALERT_4_G | Incorrectly? Oriented X(sp2)-Methyl Moiety C12 Check | |
| PLAT770_ALERT_4_G | Number of Unusual/Non-Standard Labels | 3 Note | |
| PLAT790_ALERT_4_G | Centre of Gravity not Within Unit Cell: Resd. # 2 Note | |
| PLAT977_ALERT_2_C | Check Negative Difference Density on H23A | -0.37 eA-3 | |

| Alert level G | Test Name | Alert Type | Alert Level | Description |
|---------------|-----------|------------|-------------|-------------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 3 Note | |
| PLAT072_ALERT_2_G | SHEXL First Parameter in WGHT Unusually Large | 0.11 Report | |
| PLAT083_ALERT_2_G | SHEXL Second Parameter in WGHT Unusually Large | 6.79 Why ? | |
| PLAT172_ALERT_4_G | The CIF-Embedded .res File Contains DFIX Records | 2 Report | |
| PLAT242_ALERT_2_C | Low ‘MainMol’ Ueq as Compared to Neighbors of C1 Check | |
| PLAT244_ALERT_4_G | Low ‘Solvent’ Ueq as Compared to Neighbors of P34 Check | |
| PLAT380_ALERT_4_G | Incorrectly? Oriented X(sp2)-Methyl Moiety C12 Check | |
| PLAT770_ALERT_4_G | Number of Unusual/Non-Standard Labels | 3 Note | |
| PLAT790_ALERT_4_G | Centre of Gravity not Within Unit Cell: Resd. # 2 Note | |
| PLAT977_ALERT_2_C | Check Negative Difference Density on H23A | -0.37 eA-3 | |

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0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
The following ALERTS were generated. Each ALERT has the format
\[ \text{test-name_ALERT_alert-type_alert-level} \].
Click on the hyperlinks for more details of the test.

**Alert level A**

Datablock: cu652

Bond precision: \( \text{C-C} = 0.0098 \text{ Å} \)  
Wavelength=1.54184

Cell:
- \( a = 10.4749(4) \)  
- \( b = 11.7911(4) \)  
- \( c = 15.3720(8) \)  
- \( \alpha = 80.006(4) \)  
- \( \beta = 70.269(4) \)  
- \( \gamma = 64.035(4) \)

Temperature: 150 K

Calculated
- Volume: 1606.00(13)
- Space group: P -1
- Hall group: -P 1
- Moiety formula: \( \text{C}_{25} \text{H}_{31} \text{N}_{5} \text{O}_{3} \text{P} \text{Ru}, \text{F}_{5} \text{P} \text{O}, \text{C}_{4} \text{H}_{9} \text{O} \)
- Sum formula: \( \text{C}_{29} \text{H}_{40} \text{F}_{5} \text{N}_{5} \text{O}_{4} \text{P}_{2} \text{Ru} \)
- Mr: 780.67
- \( \text{Dx},g \text{ cm}^{-3} \): 1.614
- \( \text{Z} \): 2
- \( \text{Mu (mm}^{-1} \text{)} \): 5.537
- \( F_{000} \): 800.0
- \( F_{000'} \): 803.71
- \( h,k,l_{\text{max}} \): 12,14,18
- \( N_{\text{ref}} \): 6106
- \( T_{\text{min}},T_{\text{max}} \): 0.304,0.330

Reported
- Volume: 1606.00(13)
- Space group: P -1
- Hall group: -P 1
- Moiety formula: \( \text{C}_{25} \text{H}_{31} \text{N}_{5} \text{O}_{3} \text{P} \text{Ru}, \text{F}_{5} \text{P} \text{O}, \text{C}_{4} \text{H}_{9} \text{O} \)
- Sum formula: \( \text{C}_{29} \text{H}_{40} \text{F}_{5} \text{N}_{5} \text{O}_{4} \text{P}_{2} \text{Ru} \)
- Mr: 780.67
- \( \text{Dx},g \text{ cm}^{-3} \): 1.614
- \( \text{Z} \): 2
- \( \text{Mu (mm}^{-1} \text{)} \): 5.537
- \( F_{000} \): 800.0
- \( F_{000'} \): 803.71
- \( h,k,l_{\text{max}} \): 12,14,18
- \( N_{\text{ref}} \): 5290
- \( T_{\text{min}},T_{\text{max}} \): 0.368,1.000

Correction method: # Reported T Limits: \( T_{\text{min}}=0.368 \text{ } T_{\text{max}}=1.000 \)
AbsCorr = MULTI-SCAN

Data completeness: 0.866  
Theta(max)= 70.049

\( R(\text{reflections})= 0.0570( 4971) \)  
\( wR2(\text{reflections})= 0.1599( 5290) \)

\( S = 1.083 \)  
\( N_{\text{par}}= 462 \)
Alert level B
PLAT911_ALERT_3_B Missing FCF Refl Between Thmin & STh/L= 0.600 751 Report

Alert level C
CRYSC01_ALERT_1_C The word below has not been recognised as a standard identifier.
dull
PLAT222_ALERT_3_C NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range 4.7 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference P1 --F6 . 0.22 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P1 --F7 . 0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P1 --F2A . 0.22 Ang.
PLAT243_ALERT_4_C High ‘Solvent’ Ueq as Compared to Neighbors of C41 Check
PLAT243_ALERT_4_C High ‘Solvent’ Ueq as Compared to Neighbors of C43 Check
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor .... 2.2 Note
PLAT260_ALERT_2_C Large Average Ueq of Residue Including P1 0.125 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ............... 0.00976 Ang.
PLAT362_ALERT_2_C Short C(sp3)-C(sp2) Bond C40 - C41 . 1.41 Ang.
PLAT918_ALERT_3_C Reflection(s) with I(obs) much Smaller I(calc) . 1 Check
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.57A From P1 -1.58 eA-3
PLAT972_ALERT_2_C Check Calcd Resid. Dens. 0.58A From P1 -1.54 eA-3

Alert level G
PLAT042_ALERT_1_G Calc. and Reported MoietyFormula Strings Differ Please Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large 0.11 Report
PLAT154_ALERT_1_G The s.u.’s on the Cell Angles are Equal ..(Note) 0.004 Degree
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. 1 Note
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) P1 --F1 . 6.8 s.u.
PLAT231_ALERT_4_G Hirshfeld Test (Solvent) P1 --F2 . 6.0 s.u.
PLAT244_ALERT_4_G Low ‘Solvent’ Ueq as Compared to Neighbors of P1 Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2 ) 50% Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3 ) 20% Note
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H44A ..H43D . 2.11 Ang.
PLAT412_ALERT_2_G Short Intra XH3 .. XHn H44B ..H43C . 2.09 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact F7 ..C13 . 2.96 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact F7 ..C13 . 2.96 Ang.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 65 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 1 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ........... 2.0 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

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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.

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**PLATON version of 05/12/2020; check.def file version of 05/12/2020**
Datablock cu420 - ellipsoid plot

PLATON - Feb 16 10:33:50 2021 - (51220)

Z 153 cu420 P 1 21/n 1 R = 0.06 RES = 0 -57 X
