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: nzx03

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Bond precision:  C-C = 0.0099 A          Wavelength=0.71073

Cell:          a=18.5753(9)      b=18.6769(9)     c=20.2553(10)
               alpha=83.513(4)   beta=85.582(4)   gamma=62.139(5)
Temperature:   150 K
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	Calculated	Reported
Volume	6170.5(6)	6170.5(6)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C115 H105 Ag3 P8 Ru, 2(B F4), 5(C4 H8 O)	?
Sum formula	C135 H145 Ag3 B2 F8 O5 P8 Ru	C135 H145 Ag3 B2 F8 O5 P8 Ru
Mr	2693.58	2693.56
Dx,g cm-3	1.450	1.450
Z	2	2
Mu (mm-1)	0.759	0.759
F000	2764.0	2764.0
F000’	2758.75	
h,k,lmax	24,24,26	24,24,26
Nref	30440	26131
Tmin,Tmax	0.841,0.970	0.823,1.000
Tmin’	0.749	

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Correction method= # Reported T Limits: Tmin=0.823 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.858          Theta(max)= 28.219

R(reflections)= 0.0575( 17265)    wR2(reflections)= 0.1518( 26131)

S = 1.044                 Npar= 1497
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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

PLAT213_ALERT_2_A Atom C76A has ADP max/min Ratio ..... 12.9 prolat

Author Response: The atom in question is part of a disordered phenyl ring.

Alert level B

PLAT029_ALERT_3_B _diffrn_measured_fraction_theta_full Low ..... 0.946 Note
PLAT364_ALERT_2_B Short C(sp3)-C(sp) Bond C3 - C4 .. 1.23 Ang.

Alert level C

PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ..... 5 Check
PLAT213_ALERT_2_C Atom C72A has ADP max/min Ratio ..... 3.1 prolat

Author Response: The atom in question is part of a disordered phenyl ring.

PLAT213_ALERT_2_C Atom C73A has ADP max/min Ratio ..... 4.0 prolat

Author Response: The atom in question is part of a disordered phenyl ring.

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 4.2 Ratio
PLAT223_ALERT_4_C Large Solvent/Anion H Ueq(max)/Ueq(min) ..... 4.0 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C67 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C131 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C133 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of C138 Check
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of O139 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C132 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C141 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C142 Check
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C143 Check
PLAT331_ALERT_2_C Small Average Phenyl C-C Dist. C71B -C76B 1.36 Ang.
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00989 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C140 - C141 .. 1.43 Ang.
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C141 - C142 .. 1.43 Ang.
PLAT373_ALERT_2_C Long C(sp)-C(sp) Bond C2 - C3 .. 1.36 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact H13J .. H15C .. 2.09 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact H15P .. H61 .. 2.13 Ang.

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 9 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 1 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 10.87 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records 2 Report
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 8 Report
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of B119 Check
PLAT244_ALERT_4_G Low 'Solvent' Ueq as Compared to Neighbors of B124 Check
PLAT301_ALERT_3_G Main Residue Disorder ..... Percentage = 5 Note
PLAT302_ALERT_4_G Anion/Solvent Disorder ..... Percentage = 14 Note

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PLAT304_ALERT_4_G Non-Integer Number of Atoms (   7.15) in Resd. #          8 Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms (   5.85) in Resd. #          9 Check
PLAT343_ALERT_2_G Unusual sp3      Angle Range in Main Residue for     C4     Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety .....        C20 Check
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          8 Note
             C4 H8 O
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd.  #          9 Note
             C4 H8 O
PLAT793_ALERT_4_G The Model has Chirality at C4      (Centro SPGR)          R Verify
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        11 Note
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   1 ALERT level A = Most likely a serious problem - resolve or explain
   2 ALERT level B = A potentially serious problem, consider carefully
  21 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  17 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  16 ALERT type 2 Indicator that the structure model may be wrong or deficient
   5 ALERT type 3 Indicator that the structure quality may be low
  20 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
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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*, 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 19/11/2015; check.def file version of 17/11/2015

Datablock nzx03 - ellipsoid plot