checkCIF/PLATON report

Structure factors have been supplied for datablock(s) br832

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: br832

Bond precision: C-C = 0.0254 A Wavelength=0.71073

Cell: a=20.083(4) b=34.038(8) c=37.711(8)
alpha=90 beta=90 gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	25779(10)	25779(10)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C115 H105 Ag3 P8 Ru, 2(B F4)	C115 H105 Ag3 P8 Ru, 2(B F4)
Sum formula	C115 H105 Ag3 B2 F8 P8 Ru	C115 H105 Ag3 B2 F8 P8 Ru
Mr	2333.06	2333.04
Dx,g cm-3	1.202	1.202
Z	8	8
Mu (mm-1)	0.714	0.714
F000	9456.0	9456.0
F000’	9434.24	
h,k,lmax	24,40,45	23,40,44
Nref	23117	22892
Tmin,Tmax	0.918,0.958	0.670,0.840
Tmin’	0.879	

Correction method= # Reported T Limits: Tmin=0.670 Tmax=0.840
AbsCorr = MULTI-SCAN

Data completeness= 0.990 Theta(max)= 25.165

R(reflections)= 0.1230(5506) wR2(reflections)= 0.3320(22892)

S = 0.844 Npar= 1240

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

PLAT026_ALERT_3_A Ratio Observed / Unique Reflections too Low .... 24 %
PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure ! Info

Author Response: Attempts to locate solvent molecules were not successful. The program Squeeze was used to effectively remove any electron density.

Alert level B

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0254 Ang.

Alert level C

RFACG01_ALERT_3_C The value of the R factor is > 0.10
R factor given 0.123
RFACR01_ALERT_3_C The value of the weighted R factor is > 0.25
Weighted R factor given 0.332
PLAT082_ALERT_2_C High R1 Value ..... 0.12 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ..... 0.33 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density .... 3.00 Report
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 3.4 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for P7 -- C711 .. 5.3 su
PLAT234_ALERT_4_C Large Hirshfeld Difference Ru1 -- C102 .. 0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P8 -- C811 .. 0.18 Ang.
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C214 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C226 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C312 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C314 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C321 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C423 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C425 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C515 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C524 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C612 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C615 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C623 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C816 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C111 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C311 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C313 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C422 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C516 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C611 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C614 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C622 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C811 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C815 Check
PLAT373_ALERT_2_C Long C(sp)-C(sp) Bond C2 - C3 ... 1.38 Ang.
PLAT731_ALERT_1_C Bond Calc 1.39(6), Rep 1.395(18) ..... 3 su-Rat
B2 -F22 1.555 1.555 ..... Bond # 264 Check
PLAT732_ALERT_1_C Angle Calc 110(4), Rep 109.9(17) ..... 2.35 su-Rat
F22 -B2 -F23 1.555 1.555 1.555 # 500

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PLAT732_ALERT_1_C Angle   Calc      109(4), Rep   108.7(17) ......       2.35 su-Rat
             F22  -B2   -F24     1.555   1.555   1.555      #       501
PLAT732_ALERT_1_C Angle   Calc      110(4), Rep   109.6(18) ......       2.22 su-Rat
             F23  -B2   -F24     1.555   1.555   1.555      #       502
PLAT732_ALERT_1_C Angle   Calc      113(4), Rep   113.2(18) ......       2.22 su-Rat
             F22  -B2   -F21     1.555   1.555   1.555      #       503
PLAT732_ALERT_1_C Angle   Calc      110(4), Rep   110.1(17) ......       2.35 su-Rat
             F23  -B2   -F21     1.555   1.555   1.555      #       504
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......    105.410 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.464 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     17.037 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      6.351 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.734 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.403 Check
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L=  0.598        216 Report
PLAT971_ALERT_2_C Check Calcd Residual Density  1.45A From     Ag4       1.82 eA-3
PLAT971_ALERT_2_C Check Calcd Residual Density  1.64A From     Ag3       1.74 eA-3
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Alert level G

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PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.14 Report
PLAT244_ALERT_4_G Low   'Solvent' Ueq as Compared to Neighbors of         B1 Check
PLAT343_ALERT_2_G Unusual sp?      Angle Range in Main Residue for     C4     Check
PLAT432_ALERT_2_G Short Inter X...Y Contact  F21    ..  C322    ..       2.95 Ang.
PLAT432_ALERT_2_G Short Inter X...Y Contact  F24    ..  C825    ..       2.88 Ang.
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............       2991 Note
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
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   2 ALERT level A = Most likely a serious problem - resolve or explain
   1 ALERT level B = A potentially serious problem, consider carefully
  48 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   7 ALERT level G = General information/check it is not something unexpected

   6 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  35 ALERT type 2 Indicator that the structure model may be wrong or deficient
  13 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   1 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 21/06/2015; check.def file version of 21/06/2015

Datablock br832 - ellipsoid plot