checkCIF/PLATON report

Structure factors have been supplied for datablock(s) br839

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: br839

Bond precision: C-C = 0.0199 A Wavelength=0.71073

Cell: a=19.647(3) b=34.033(6) c=37.872(5)
alpha=90 beta=90 gamma=90
Temperature: 150 K

	Calculated	Reported
Volume	25323(7)	25323(7)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C115 H105 Cu3 P8 Ru, 2(B F4)	C115 H105 Cu3 P8 Ru, 2(B F4)
Sum formula	C115 H105 B2 Cu3 F8 P8 Ru	C115 H105 B2 Cu3 F8 P8 Ru
Mr	2200.10	2200.05
Dx,g cm-3	1.154	1.154
Z	8	8
Mu (mm-1)	0.767	0.767
F000	9024.0	9024.0
F000’	9031.16	
h,k,lmax	23,40,45	23,40,44
Nref	22316	22316
Tmin,Tmax	0.885,0.948	0.440,0.780
Tmin’	0.885	

Correction method= # Reported T Limits: Tmin=0.440 Tmax=0.780
AbsCorr = MULTI-SCAN

Data completeness= 1.000 Theta(max)= 25.000

R(reflections)= 0.1352(14557) wR2(reflections)= 0.3442(22316)

S = 1.060 Npar= 1239

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

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RFACG01_ALERT_3_C  The value of the R factor is > 0.10
           R factor given   0.135
RFACR01_ALERT_3_C  The value of the weighted R factor is > 0.25
           Weighted R factor given   0.344
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.140
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 .........      0.140 Report
PLAT082_ALERT_2_C High R1 Value ..................................       0.14 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.34 Report
PLAT220_ALERT_2_C Large Non-Solvent  C     Ueq(max)/Ueq(min) Range        5.2 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference P3     --  C30     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P4     --  C30     ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference P4     --  C421    ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C102   --  C103    ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C213   --  C214    ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C311   --  C312    ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C311   --  C316    ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C314   --  C315    ..       0.20 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C315   --  C316    ..       0.23 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C321   --  C322    ..       0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C412   --  C413    ..       0.19 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C515   --  C516    ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C611   --  C616    ..       0.16 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C621   --  C622    ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C622   --  C623    ..       0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C815   --  C816    ..       0.18 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C825   --  C826    ..       0.18 Ang.
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C114 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C313 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C315 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C324 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C616 Check
PLAT241_ALERT_2_C High      Ueq as Compared to Neighbors for .....       C825 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 .....       C314 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
PLAT332_ALERT_2_C Large Phenyl C-C Range           C411   -C416         0.21 Ang.
PLAT342_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0199 Ang.
PLAT373_ALERT_2_C Long   C(sp)-C(sp)   Bond  C2     -   C3     ...      1.36 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......     15.203 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      3.779 Check
PLAT906_ALERT_3_C Large K value in the Analysis of Variance ......      2.119 Check
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Alert level G

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PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT Unusually Large.       0.13 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.     463.93 Why ?
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
PLAT606_ALERT_4_G VERY LARGE Solvent Accessible VOID(S) in Structure        ! Info
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Author Response: Attempts to locate solvent molecules resulted in several molecules with huge U(eq) values and with R~.14. Use of the program Squeeze resulted in much lower residuals.

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PLAT860_ALERT_3_G Number of Least-Squares Restraints .............        598 Note
PLAT869_ALERT_4_G ALERTS Related to the use of SQUEEZE Suppressed           ! Info
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) still          33 %
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities .......     Please Check
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   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  40 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   9 ALERT level G = General information/check it is not something unexpected

   0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  17 ALERT type 2 Indicator that the structure model may be wrong or deficient
  11 ALERT type 3 Indicator that the structure quality may be low
  20 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 br839 - ellipsoid plot