

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rucb8pm

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: rucb8pm

Bond precision:	C-C = 0.0162 A	Wavelength=0.71073	
Cell:	a=18.467(11)	b=15.515(9)	c=18.611(11)
	alpha=90	beta=100.170(11)	gamma=90
Temperature:	110 K		
	Calculated	Reported	
Volume	5249(5)	5249(5)	
Space group	P 21/c	P 21/c	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	C44 H45 B8 Cl O P2 Ru, C0.67 H1.33 Cl1.33, 1.333(C H2 Cl2)	C44 H45 B8 Cl O P2 Ru, 2(C H2 Cl2)	
Sum formula	C46 H49 B8 Cl5 O P2 Ru	C46 H49 B8 Cl5 O P2 Ru	
Mr	1044.60	1044.59	
Dx, g cm-3	1.322	1.322	
Z	4	4	
Mu (mm-1)	0.647	0.647	
F000	2128.0	2128.0	
F000'	2127.25		
h, k, lmax	22, 19, 22	22, 19, 22	
Nref	10305	10275	
Tmin, Tmax	0.780, 0.845	0.560, 0.928	
Tmin'	0.733		

Correction method= # Reported T Limits: Tmin=0.560 Tmax=0.928

AbsCorr = MULTI-SCAN

Data completeness= 0.997

Theta(max)= 25.999

R(reflections)= 0.0987(5005)

wR2(reflections)=
0.2767(10275)

S = 1.009

Npar= 602

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

PLAT971_ALERT_2_B Check Calcd Resid. Dens. 1.04Ang From Ru1

2.82 eA-3

Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.

Absorption correction given as multi-scan

RINTA01_ALERT_3_C The value of Rint is greater than 0.12

Rint given 0.126

PLAT020_ALERT_3_C The Value of Rint is Greater Than 0.12	0.126 Report
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..	49% Check
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ	Please Check
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25)	0.28 Report
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density	2.82 Report
PLAT214_ALERT_2_C Atom ClS (Anion/Solvent) ADP max/min Ratio	4.1 oblate
PLAT234_ALERT_4_C Large Hirshfeld Difference P2 --B3 .	0.17 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference C21 --C22 .	0.21 Ang.
PLAT234_ALERT_4_C Large Hirshfeld Difference B8 --B9 .	0.16 Ang.
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cl5S	0.112 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cl1S	0.130 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including Cl3S	0.113 Check
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds	0.01616 Ang.
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ...	-5.000 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600	17 Report
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.20Ang From Ru1	2.18 eA-3
PLAT971_ALERT_2_C Check Calcd Resid. Dens. 1.33Ang From Ru1	2.09 eA-3
PLAT973_ALERT_2_C Check Calcd Positive Resid. Density on Ru1	1.18 eA-3

Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large	50.00 Why ?
PLAT171_ALERT_4_G The CIF-Embedded .res File Contains EADP Records	2 Report
PLAT300_ALERT_4_G Atom Site Occupancy of Cl5S Constrained at	0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl6S Constrained at	0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl5' Constrained at	0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl6' Constrained at	0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of C3S Constrained at	0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3SA Constrained at	0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3SB Constrained at	0.5 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3SC Constrained at	0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of H3SD Constrained at	0.1667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl1S Constrained at	0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl2S Constrained at	0.6667 Check
PLAT300_ALERT_4_G Atom Site Occupancy of ClS Constrained at	0.6667 Check

PLAT300_ALERT_4_G Atom Site Occupancy of H1SA	Constrained at	0.6667	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H1SB	Constrained at	0.6667	Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl3S	Constrained at	0.6667	Check
PLAT300_ALERT_4_G Atom Site Occupancy of Cl4S	Constrained at	0.6667	Check
PLAT300_ALERT_4_G Atom Site Occupancy of C2S	Constrained at	0.6667	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2SA	Constrained at	0.6667	Check
PLAT300_ALERT_4_G Atom Site Occupancy of H2SB	Constrained at	0.6667	Check
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 2)		100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 3)		100%	Note
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd 4)		100%	Note
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 2)		3.33	Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 3)		3.33	Check
PLAT304_ALERT_4_G Non-Integer Number of Atoms in (Resd 4)		3.33	Check
PLAT343_ALERT_2_G Unusual Angle Range in Main Residue for C2			Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels		8	Note
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # C H2 Cl2		4	Note
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).		1	Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600		13	Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF		1	Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File		18	Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity		4.4	Low
PLAT965_ALERT_2_G The SHELXL WEIGHT Optimisation has not Converged			Please Check
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..		52.0	Degree
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.		0	Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
 1 **ALERT level B** = A potentially serious problem, consider carefully
 20 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 38 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 14 ALERT type 2 Indicator that the structure model may be wrong or deficient
 10 ALERT type 3 Indicator that the structure quality may be low
 32 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.

