

Datablock: Ru_acac

Bond precision: C-C = 0.0109 Å Wavelength=0.71075
Cell: a=8.5579(9) b=9.9459(12) c=14.7303(15)
alpha=90 beta=98.009(7) gamma=90
Temperature: 103 K

	Calculated	Reported
Volume	1241.6(2)	1241.6(2)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C12 H15 Cl O2 Ru	C12 H15 Cl O2 Ru
Sum formula	C12 H15 Cl O2 Ru	C12 H15 Cl O2 Ru
Mr	327.76	327.76
Dx, g cm-3	1.753	1.753
Z	4	4
Mu (mm-1)	1.460	1.460
F000	656.0	656.0
F000'	651.75	
h,k,lmax	11,12,19	11,12,19
Nref	2828	2823
Tmin,Tmax	0.869,0.899	0.924,0.981
Tmin'	0.603	

Correction method= # Reported T Limits: Tmin=0.924 Tmax=0.981
AbsCorr = NUMERICAL
Data completeness= 0.998 Theta(max)= 27.450
R(reflections)= 0.0668(1972) wR2(reflections)= 0.1159(2823)
S = 1.063 Npar= 148

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

PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.01091 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	19.038 Check
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.536 Check
PLAT977_ALERT_2_C	Check Negative Difference Density on H7B	-0.31 eA-3
PLAT978_ALERT_2_C	Number C-C Bonds with Positive Residual Density.	0 Info

Alert level G

PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	5.11 Why ?
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C7 Check
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	3 Note
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	2 Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF	1 Note

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 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
2 ALERT type 4 Improvement, methodology, query or suggestion
0 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.

PLATON version of 19/10/2018; check.def file version of 15/10/2018

Datablock Ru_acac - ellipsoid plot

