

No syntax errors found.
Please wait while processing

[CIF dictionary](#)
[Interpreting this report](#)

Datablock: 33_02_080b

Bond precision:	C-C = 0.0058 Å	Wavelength=0.71075
Cell:	a=11.5108(13) b=11.7477(12) c=17.714(2)	
	alpha=77.954(5) beta=82.044(5) gamma=68.932(4)	
Temperature:	143 K	
	Calculated	Reported
Volume	2180.8(4)	2180.7(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C49 H48 Al Cl2 O2 P2 Rh	C49 H48 Al Cl2 O2 P2 Rh
Sum formula	C49 H48 Al Cl2 O2 P2 Rh	C49 H48 Al Cl2 O2 P2 Rh
Mr	931.60	931.66
Dx, g cm-3	1.419	1.419
Z	2	2
Mu (mm-1)	0.647	0.646
F000	960.0	960.0
F000'	959.16	
h,k,lmax	13,13,21	13,13,21
Nref	7698	7551
Tmin,Tmax	0.897,0.937	0.770,0.937
Tmin'	0.890	
Correction method=	# Reported T Limits: Tmin=0.770	
Tmax=0.937 AbsCorr =	MULTI-SCAN	
Data completeness=	0.981	Theta(max)= 25.030
R(reflections)=	0.0400(6634)	wR2(reflections)= 0.1291(7551)
S =	1.166	Npar= 514

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

PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	3.8 Ratio
PLAT232_ALERT_2_C	Hirshfeld Test Diff (M-X) Rh1 --P2 .	5.3 s.u.

● Alert level G

CHEMS02_ALERT_1_G	Please check that you have entered the correct _publ_requested_category classification of your compound; FI or CI or EI for inorganic; FM or CM or EM for metal-organic; FO or CO or EO for organic. From the CIF: _publ_requested_category CHOOSE FI FM FO CI CM CO or A From the CIF: _chemical_formula_sum :C49 H48 Al1 Cl2 O2 P2 Rh1	
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !
PLAT794_ALERT_5_G	Tentative Bond Valency for Al1 (III) .	3.00 Info
PLAT882_ALERT_1_G	No Datum for _diffrn_reflns_av_unetI/netI	Please Do !

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

- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
2 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

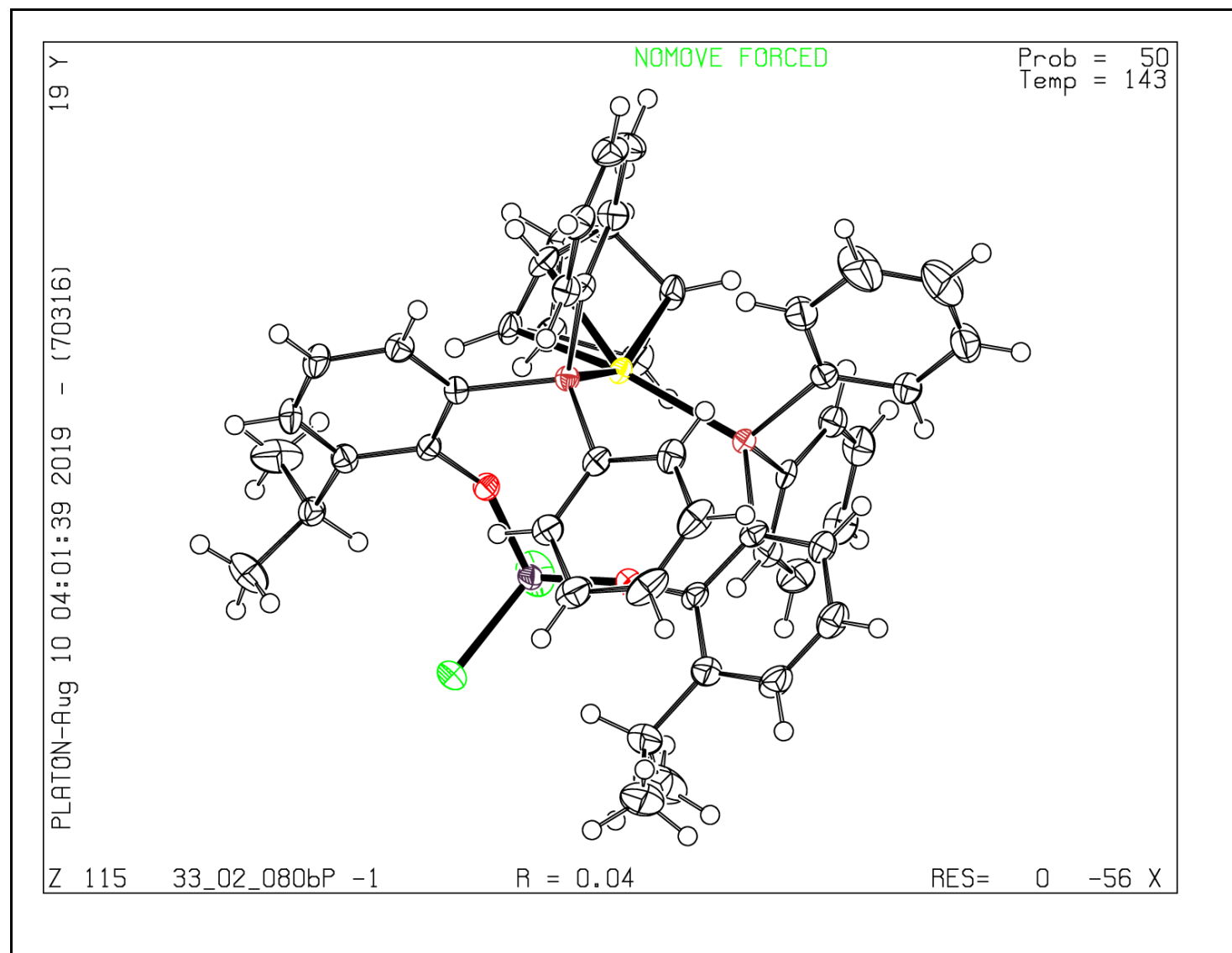
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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 07/08/2019; check.def file version of 30/07/2019

Datablock 33_02_080b - ellipsoid plot



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