

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) _33_05_032a

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: _33_05_032a

Bond precision: C-C = 0.0078 Å Wavelength=0.71075

Cell: a=21.467(2) b=23.846(3) c=22.560(3)
 alpha=90 beta=90 gamma=90
Temperature: 143 K

	Calculated	Reported
Volume	11549(2)	11549(2)
Space group	P b c n	P b c n
Hall group	-P 2n 2ab	-P 2n 2ab
Moiety formula	C105 H105.39 Al2 N4 O4 P4 Rh2, C10, C6 H6, 2(C5 H8)	C105 H105.395 Al2 N4 O4 P4 Rh2, C6 H6, C10 H16, C10
Sum formula	C131 H127.39 Al2 N4 O4 P4 Rh2	C131 H127.39 Al2 N4 O4 P4 Rh2
Mr	2205.42	2205.42
Dx, g cm ⁻³	1.268	1.268
Z	4	4
Mu (mm ⁻¹)	0.411	0.411
F000	4597.6	4598.0
F000'	4592.17	
h,k,lmax	27,30,29	27,29,29
Nref	13249	13125
Tmin,Tmax	0.966,0.976	0.863,1.000
Tmin'	0.925	

Correction method= # Reported T Limits: Tmin=0.863 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.991 Theta(max)= 27.486

R(reflections)= 0.0467(11795) wR2(reflections)= 0.1163(13125)

S = 1.104 Npar= 680

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

PLAT910_ALERT_3_B Missing # of FCF Reflection(s) Below Theta(Min). 20 Note

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

PLAT094_ALERT_2_C	Ratio of Maximum / Minimum Residual Density	2.32	Report
PLAT202_ALERT_3_C	Isotropic non-H Atoms in Anion/Solvent	5	Check
	C5 C6 C7 C8 C9		
PLAT220_ALERT_2_C	Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range	4.4	Ratio
PLAT222_ALERT_3_C	Non-Solv. Resd 1 H Uiso(max)/Uiso(min) Range	5.5	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C8	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C01N	Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C01X	Check
PLAT260_ALERT_2_C	Large Average Ueq of Residue Including	C1	0.181 Check
PLAT331_ALERT_2_C	Small Aver Phenyl C-C Dist C00Y -C01L_c	1.36	Ang.
PLAT360_ALERT_2_C	Short C(sp3)-C(sp3) Bond C7 - C7_b	1.37	Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	5.030	Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	25	Report

Alert level G

PLAT042_ALERT_1_G	Calc. and Reported MoietyFormula Strings Differ	Please	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...	Please	Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	15.02	Why ?
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C01M --C01S	13.0	s.u.
PLAT300_ALERT_4_G	Atom Site Occupancy of H20A Constrained at	0.5	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H20B Constrained at	0.5	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 1)	5%	Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in Resd 1	226.39	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C21	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C22	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C5	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C6	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C7	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C8	Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C9	Check
PLAT344_ALERT_2_G	Unusual sp? Angle Range in Solvent/Ion for	C1	Check
PLAT344_ALERT_2_G	Unusual sp? Angle Range in Solvent/Ion for	C01V	Check
PLAT344_ALERT_2_G	Unusual sp? Angle Range in Solvent/Ion for	C01X	Check
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C00C - C20	1.53	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C00C - C21	1.54	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C00C - C22_a	1.54	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C00X - C01N	1.52	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C01A - C01M	1.50	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C5 - C6	1.63	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C5 - C9_b	1.72	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C6 - C7	1.67	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C6 - C7_b	1.62	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C7 - C8	1.60	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C8 - C9	1.65	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C1 - C01V	1.70	Ang.
PLAT367_ALERT_2_G	Long? C(sp?)-C(sp?) Bond C01T - C01X	1.72	Ang.

PLAT432_ALERT_2_G Short Inter X...Y Contact	C8	..C2	2.48 Ang.
		x,y,z =	1_555 Check
PLAT432_ALERT_2_G Short Inter X...Y Contact	C9	..C2	2.63 Ang.
		x,y,z =	1_555 Check
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels		116 Note
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C01T	--C01X		1.72 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C01V	--C1		1.70 Ang.
PLAT773_ALERT_2_G Check long C-C Bond in CIF: C9	--C5		1.72 Ang.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=	0.600		36 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF		2 Note
PLAT933_ALERT_2_G Number of OMIT Records in Embedded .res File	...		1 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.			2 Info

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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 39 ALERT type 2 Indicator that the structure model may be wrong or deficient
 7 ALERT type 3 Indicator that the structure quality may be low
 6 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.

