

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) P21c_a_sq_sq

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: P21c_a_sq_sq

Bond precision: C-C = 0.0310 Å Wavelength=1.54178

Cell: a=29.175 (3) b=26.200 (2) c=28.400 (2)
 alpha=90 beta=113.682 (4) gamma=90

Temperature: 150 K

	Calculated	Reported
Volume	19880 (3)	19881 (3)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C156 H146 N8 O12 Rh6 [+ solvent]	?
Sum formula	C156 H146 N8 O12 Rh6 [+ solvent]	C156 H146 N8 O12 Rh6
Mr	2942.28	2942.26
Dx, g cm ⁻³	0.983	0.983
Z	4	4
Mu (mm ⁻¹)	4.285	4.285
F000	6016.0	6016.0
F000'	6032.82	
h, k, lmax	29, 26, 28	29, 26, 28
Nref	21415	21140
Tmin, Tmax	0.628, 0.651	
Tmin'	0.492	

Correction method= Not given

Data completeness= 0.987 Theta(max)= 51.089

R(reflections)= 0.1778 (6108)

wR2(reflections)=
0.4505 (21140)

S = 1.109

Npar= 1351

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 A

THETM01_ALERT_3_A The value of sine(theta_max)/wavelength is less than 0.550

Calculated sin(theta_max)/wavelength = 0.5047

Author Response: crystal diffracted weakly, the diffraction limit can only reach 1.35

PLAT026_ALERT_3_A Ratio Observed / Unique Reflections (too) Low .. 29% Check

Author Response: crystal diffracted weakly, the diffraction limit can only reach 1.35

PLAT242_ALERT_2_A Low 'MainMol' Ueq as Compared to Neighbors of Rh1 Check

Author Response: stucture disordered there

PLAT242_ALERT_2_A Low 'MainMol' Ueq as Compared to Neighbors of Rh3 Check

Author Response: stucture disordered there

PLAT242_ALERT_2_A Low 'MainMol' Ueq as Compared to Neighbors of Rh6 Check

Author Response: stucture disordered there

Alert level B

PLAT082_ALERT_2_B High R1 Value 0.18 Report

PLAT084_ALERT_3_B High wR2 Value (i.e. > 0.25) 0.45 Report

PLAT220_ALERT_2_B NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 8.6 Ratio

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C1_8 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C2_8 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C3_8 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C4_8 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C5_8 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C1_11 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C2_11 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C3_11 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C4_11 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C5_11 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C1_12 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C2_12 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C3_12 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C4_12 Check

PLAT241_ALERT_2_B High 'MainMol' Ueq as Compared to Neighbors of C5_12 Check

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of Rh5 Check

Author Response: stucture disordered there

PLAT242_ALERT 2 B Low 'MainMol' Ueq as Compared to Neighbors of 04_5 Check

Author Response: stucture disordered there

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of N4_2 Check

Author Response: structure disordered there

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of N1_4 Check

Author Response: stucture disordered there

PLAT242_ALERT_2_B Low 'MainMol' Ueq as Compared to Neighbors of N4_4 Check

Author Response: structure disordered there

PLAT260_ALERT_2_B	Large Average Ueq of Residue Including	Rh1	0.544	Check
PLAT342_ALERT_3_B	Low Bond Precision on C-C Bonds		0.03099	Ang.
PLAT369_ALERT_2_B	Long C(sp2)-C(sp2) Bond C26_4 - C29_4	.	1.57	Ang.
PLAT410_ALERT_2_B	Short Intra H...H Contact H15_2 ..H22_2	.	1.84	Ang.
		x, y, z =	1_555	Check
PLAT413_ALERT_2_B	Short Inter XH3 .. XHn H8B_1 ..H7B_6	.	1.91	Ang.
		x, 3/2-y, 1/2+z =	4_576	Check
PLAT413_ALERT_2_B	Short Inter XH3 .. XHn H8B_1 ..H7C_6	.	1.97	Ang.
		x, 3/2-y, 1/2+z =	4_576	Check

Alert level C

PLAT052_ALERT_1_C	Info on Absorption Correction Method	Not Given	Please Do !
PLAT213_ALERT_2_C	Atom Rh4	has ADP max/min Ratio	3.2 prolat
PLAT213_ALERT_2_C	Atom O3_5	has ADP max/min Ratio	3.1 prolat
PLAT213_ALERT_2_C	Atom C1_3	has ADP max/min Ratio	3.2 prolat
PLAT213_ALERT_2_C	Atom C2_3	has ADP max/min Ratio	3.7 prolat
PLAT213_ALERT_2_C	Atom C3_3	has ADP max/min Ratio	3.6 prolat
PLAT213_ALERT_2_C	Atom C4_3	has ADP max/min Ratio	3.4 prolat
PLAT213_ALERT_2_C	Atom C8_3	has ADP max/min Ratio	3.2 prolat
PLAT213_ALERT_2_C	Atom C1_6	has ADP max/min Ratio	3.2 prolat
PLAT213_ALERT_2_C	Atom C5_6	has ADP max/min Ratio	3.3 prolat
PLAT213_ALERT_2_C	Atom C10_6	has ADP max/min Ratio	3.1 prolat
PLAT213_ALERT_2_C	Atom C10_8	has ADP max/min Ratio	3.1 prolat
PLAT213_ALERT_2_C	Atom C3_12	has ADP max/min Ratio	3.1 prolat
PLAT218_ALERT_3_C	Constrained U(ij) Components(s) for C1#	.	6 Check
PLAT218_ALERT_3_C	Constrained U(ij) Components(s) for C2#	.	6 Check
PLAT218_ALERT_3_C	Constrained U(ij) Components(s) for C3#	.	6 Check
PLAT218_ALERT_3_C	Constrained U(ij) Components(s) for C4#	.	6 Check
PLAT218_ALERT_3_C	Constrained U(ij) Components(s) for C5#	.	6 Check
PLAT218_ALERT_3_C	Constrained U(ij) Components(s) for N1#	.	6 Check
PLAT218_ALERT_3_C	Constrained U(ij) Components(s) for C6#	.	6 Check

[illegible]

[illegible]

[illegible]

PLAT218_ALERT_3_C	Constrained U(ij) Components(s) for C153#	.	6	Check
PLAT218_ALERT_3_C	Constrained U(ij) Components(s) for C154#	.	6	Check
PLAT218_ALERT_3_C	Constrained U(ij) Components(s) for C155#	.	6	Check
PLAT218_ALERT_3_C	Constrained U(ij) Components(s) for C156#	.	6	Check
PLAT220_ALERT_2_C	NonSolvent Resd 1 Rh Ueq(max)/Ueq(min) Range		3.4	Ratio
PLAT222_ALERT_3_C	NonSolvent Resd 1 H Uiso(max)/Uiso(min) Range		10.0	Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		O1_5	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		O2_5	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		O3_5	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C32_2	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C2_3	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C5_3	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C1_1	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C2_1	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C3_1	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C4_1	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C5_1	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C1_6	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C2_6	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C3_6	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of		C4_6	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Rh2	Check

Author Response: stucture disordered there

PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		Rh4	Check
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Author Response: stucture disordered there

PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		O2_7	Check
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Author Response: stucture disordered there

PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		O1_9	Check
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Author Response: stucture disordered there

PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		O2_9	Check
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Author Response: stucture disordered there

PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		N1_2	Check
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Author Response: stucture disordered there

PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of		N2_2	Check
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Author Response: stucture disordered there

PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of N2_4 Check

Author Response: stucture disordered there

PLAT369_ALERT_2_C Long C(sp2)-C(sp2) Bond C26_2 - C29_2 . 1.54 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact H30_2 ..H8_5 . 2.11 Ang.
1-x,1-y,1-z = 3_666 Check
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -83.908 Report
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -9.639 Report
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.992 Report
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.505 274 Report
1 4 0, 26 7 0, -27 3 1, -27 4 1, -26 8 1, -18 20 1,
-9 25 1, -5 26 1, 2 4 1, 24 11 1, 26 4 1, 26 5 1,
-27 5 2, -27 6 2, -14 23 2, -5 0 2, -2 1 2, 14 22 2,
24 10 2, 25 7 2, 26 0 2, 26 1 2, 26 2 2, -28 1 3,
-5 26 3, -3 2 3, 0 1 3, 7 25 3, 23 3 3, 25 4 3,
25 5 3, -28 2 4, -28 3 4, -28 4 4, -20 19 4, -1 0 4,
0 26 4, 1 1 4, 1 26 4, 9 24 4, 23 10 4, 24 7 4,
25 0 4, 25 1 4, -23 16 5, -3 26 5, -2 26 5, -1 26 5,
22 2 5, 23 8 5, 24 4 5, -9 25 6, -1 1 6, 23 6 6,
-29 1 7, -26 12 7, -12 24 7, -8 25 7, 23 1 7, 23 2 7,
23 3 7, -29 0 8, -29 1 8, -7 25 8, 0 25 8, 1 25 8,
22 4 8, 22 5 8, -16 22 9, -11 24 9, -6 25 9, -5 25 9,
-4 25 9, -3 25 9, -2 25 9, -27 1 10, -19 20 10, -10 24 10,
2 24 10, 21 0 10, 21 1 10, 21 2 10, -27 1 11, -17 21 11,
-15 22 11, -9 24 11, -8 24 11, -1 24 11, 0 24 11, 20 2 11,
20 3 11, -27 0 12, -12 23 12, -5 24 12, 2 23 12, 10 19 12,
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF 4 Note
-2 1 2, -3 2 3, 0 1 3, -1 0 4,
PLAT977_ALERT_2_C Check Negative Difference Density on H32_4 . -0.33 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 168 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 179 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 120.00 Why ?
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 12 Report
PLAT174_ALERT_4_G The CIF-Embedded .res File Contains FLAT Records 2 Report
PLAT175_ALERT_4_G The CIF-Embedded .res File Contains SAME Records 4 Report
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records 2 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT187_ALERT_4_G The CIF-Embedded .res File Contains RIGU Records 3 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0200 Report
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C6_3 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C7_3 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C8_3 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C9_3 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C10_3 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C6_1 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C7_1 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C8_1 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C9_1 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C10_1 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C6_6 Check
PLAT380_ALERT_4_G Incorrectly? Oriented X(sp2)-Methyl Moiety C8_6 Check

PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C9_6	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C10_6	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C6_8	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C7_8	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C8_8	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C9_8	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C10_8	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C6_11	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C7_11	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C9_11	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C10_11	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C6_12	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C7_12	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C8_12	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C9_12	Check
PLAT380_ALERT_4_G	Incorrectly? Oriented X(sp2)-Methyl Moiety	C10_12	Check
PLAT432_ALERT_2_G	Short Inter X...Y Contact C8_1 ..C7_6 .	3.02	Ang.
	x,3/2-y,1/2+z =	4_576	Check
PLAT606_ALERT_4_G	Solvent Accessible VOID(S) in Structure	!	Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	2536	Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	!	Info
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1	Note
	1 0 0,		
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3	Note
	-1 1 6, 2 4 1, 1 1 4,		
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	3.9	Low
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	2.30	Note
	Predicted wR2: Based on SigI**2 19.55 or SHELX Weight 42.79		
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	1	Info

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

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
 75 ALERT type 2 Indicator that the structure model may be wrong or deficient
 196 ALERT type 3 Indicator that the structure quality may be low
 36 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.

