



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) rudi004

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: rudi004

Bond precision: C-C = 0.0042 Å

Wavelength=1.54178

Cell: a=11.9319(4) b=13.0302(4) c=19.2173(6)
 alpha=93.964(2) beta=98.560(1) gamma=97.140(1)
Temperature: 100 K

	Calculated	Reported
Volume	2919.90(16)	2919.90(16)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	2(C H B11 Cl11), C14 H16 Ni, 2(C7 H8)	C14 H16 Ni, 2(C H B11 Cl11), 2(C7 H8)
Sum formula	C30 H34 B22 Cl22 Ni	C30 H34 B22 Cl22 Ni
Mr	1470.98	1471.00
Dx, g cm ⁻³	1.673	1.673
Z	2	2
Mu (mm ⁻¹)	9.978	9.978
F000	1452.0	1452.0
F000'	1463.74	
h, k, lmax	14, 16, 24	14, 16, 23
Nref	11939	11733
Tmin, Tmax	0.121, 0.233	0.377, 0.754
Tmin'	0.034	

Correction method= # Reported T Limits: Tmin=0.377 Tmax=0.754
AbsCorr = MULTI-SCAN

Data completeness= 0.983

Theta(max)= 74.541

R(reflections)= 0.0385(10546)

wR2(reflections)=
0.1038(11733)

S = 1.033

Npar= 745

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

PLAT042_ALERT_1_C	Calc. and Reported MoietyFormula Strings Differ	Please Check
Calc.: 2(C H B11 Cl11), C14 H16 Ni, 2(C7 H8)		
Rep.: C14 H16 Ni, 2(C H B11 Cl11), 2(C7 H8)		
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 4)	2.3 Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 5)	2.7 Note
PLAT250_ALERT_2_C	Large U3/U1 Ratio for <U(i,j)> Tensor(Resd 6)	3.2 Note
PLAT351_ALERT_3_C	Long C-H (X0.96,N1.08A) C15 - H15 .	1.12 Ang.
PLAT351_ALERT_3_C	Long C-H (X0.96,N1.08A) C16 - H16 .	1.12 Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	47 Report
-14 3 0, 13 3 0, -14 0 1, -4 1 1, 2 2 1, 13 2 1,		
13 3 1, -4 15 1, -1 15 1, -14 -1 2, 13 3 2, -2 -3 3,		
13 2 3, -4 15 3, 13 -3 4, 13 2 4, -13 -4 5, 1 13 7,		
2-14 8, 3-14 8, -12 -5 8, 3-14 9, 3-14 10, 4-14 10,		
-9 11 10, 2-13 12, 3-13 13, 4-12 13, 8 4 14, -6 11 14,		
(17 More NOT listed: see .ckf listing file)		



Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	14 Note
PLAT003_ALERT_2_G	Number of Uiso or U(i,j) Restrained non-H-Atoms	14 Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	3 Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	5 Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	2 Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	3 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	1 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0020 Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400 Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400 Report
PLAT231_ALERT_4_G	Hirshfeld Test (Solvent) C29 --C30 .	10.5 s.u.
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 5)	100% Note
PLAT302_ALERT_4_G	Anion/Solvent/Minor-Residue Disorder (Resd 6)	100% Note
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 5)	11.93 Check
PLAT304_ALERT_4_G	Non-Integer Number of Atoms in (Resd 6)	3.07 Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C15 Check
PLAT343_ALERT_2_G	Unusual sp? Angle Range in Main Residue for	C16 Check
PLAT413_ALERT_2_G	Short Inter XH3 .. XHn H18 ..H30E .	1.81 Ang.
1-x,2-y,1-z = 2_676 Check		
PLAT432_ALERT_2_G	Short Inter X...Y Contact C19 ..C30A .	3.24 Ang.
1-x,1-y,1-z = 2_666 Check		
PLAT432_ALERT_2_G	Short Inter X...Y Contact C119 ..C30A .	3.09 Ang.
1-x,1-y,1-z = 2_666 Check		

