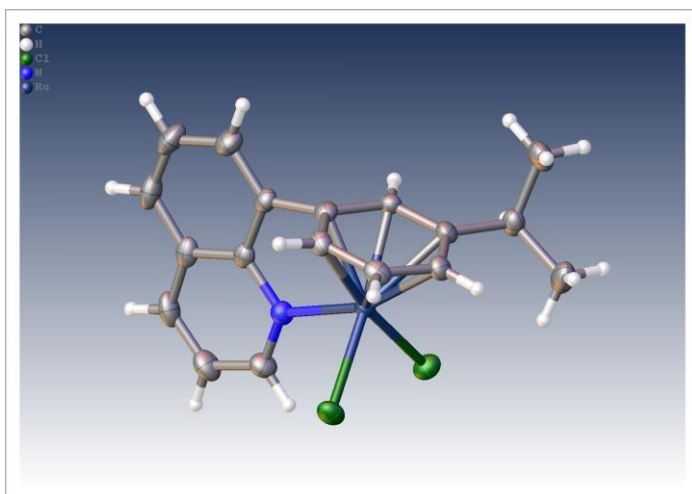


Sample ID: 03612

 $R_1 = 2.36\%$

Crystal Data and Experimental



Experimental. Single clear yellow plate-shaped crystals of **03612** were obtained. A suitable crystal $0.07 \times 0.05 \times 0.01$ mm³ was selected and placed on a MiTeGen micromount on an XtaLAB Synergy R, HyPix-Arc 100 diffractometer. The crystal was kept at a steady $T = 150.00(10)$ K during data collection. The structure was solved with the ShelXT 2018/2 (Sheldrick, 2018) structure solution program using the Intrinsic Phasing solution method and by using Olex2 (Dolomanov et al., 2009) as the graphical interface. The model was refined with version 2018/3 of ShelXL 2018/3 (Sheldrick, 2015) using Least Squares minimisation.

Crystal Data. C₁₈H₁₇NCl₂Ru, $M_r = 419.29$, monoclinic, $P2_1/c$ (No. 14), $a = 10.32170(10)$ Å, $b = 16.4107(2)$ Å, $c = 9.69320(10)$ Å, $\beta = 103.1790(10)^\circ$, $\alpha = \gamma = 90^\circ$, $V = 1598.65(3)$ Å³, $T = 150.00(10)$ K, $Z = 4$, $Z' = 1$, $\mu(\text{Cu } K\alpha) = 10.955$, 29026 reflections measured, 2926 unique ($R_{\text{int}} = 0.0484$) which were used in all calculations. The final wR_2 was 0.0565 (all data) and R_1 was 0.0236 ($I > 2(I)$).

Compound	03612
Formula	C ₁₈ H ₁₇ NCl ₂ Ru
$D_{\text{calc}} / \text{g cm}^{-3}$	1.742
μ / mm^{-1}	10.955
Formula Weight	419.29
Colour	clear yellow
Shape	plate
Size/mm ³	$0.07 \times 0.05 \times 0.01$
T/K	150.00(10)
Crystal System	monoclinic
Space Group	$P2_1/c$
$a/\text{\AA}$	10.32170(10)
$b/\text{\AA}$	16.4107(2)
$c/\text{\AA}$	9.69320(10)
$\alpha/^\circ$	90
$\beta/^\circ$	103.1790(10)
$\gamma/^\circ$	90
$V/\text{\AA}^3$	1598.65(3)
Z	4
Z'	1
Wavelength/Å	1.54184
Radiation type	Cu $K\alpha$
$\theta_{\text{min}}/^\circ$	4.399
$\theta_{\text{max}}/^\circ$	68.284
Measured Refl.	29026
Independent Refl.	2926
Reflections with $I > 2(I)$	2662
R_{int}	0.0484
Parameters	201
Restraints	0
Largest Peak	0.565
Deepest Hole	-0.399
GooF	1.050
wR_2 (all data)	0.0565
wR_2	0.0550
R_1 (all data)	0.0273
R_1	0.0236

Structure Quality Indicators

Reflections:	d min (CuKα) 2θ=136.6°	0.83	I/σ(I)	42.5	Rint m=10.19	4.84%	Full 135.4°	100
	Shift	0.001	Max Peak	0.6	Min Peak	-0.4	Goof	1.050

Experimental Extended. A clear yellow plate-shaped crystal with dimensions 0.07×0.05×0.01 mm³ was placed on a MiTeGen micromount. Data were collected using an XtaLAB Synergy R, HyPix-Arc 100 diffractometer operating at *T* = 150.00(10) K.

Data were measured using ω scans of 0.5° per frame for 0.1/0.4 s using Cu K α radiation. The diffraction pattern was indexed and the total number of runs and images was based on the strategy calculation from the program CrysAlisPro (Rigaku) The maximum resolution that was achieved was Θ = 68.284° (0.83 Å).

The diffraction pattern was indexed The diffraction pattern was indexed and the total number of runs and images was based on the strategy calculation from the program CrysAlisPro (Rigaku) and the unit cell was refined using CrysAlisPro (Rigaku, V1.171.43.127a, 2024) on 12428 reflections, 43% of the observed reflections.

Data reduction, scaling and absorption corrections were performed using CrysAlisPro (Rigaku, V1.171.43.127a, 2024). The final completeness is 100.00 % out to 68.284° in Θ . A gaussian absorption correction was performed using CrysAlisPro 1.171.43.127a (Rigaku Oxford Diffraction, 2024) Numerical absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm. The absorption coefficient μ of this material is 10.955 mm⁻¹ at this wavelength (λ = 1.542Å) and the minimum and maximum transmissions are 0.556 and 0.967.

The structure was solved and the space group *P*2₁/*c* (# 14) determined by the ShelXT 2018/2 (Sheldrick, 2018) structure solution program using Intrinsic Phasing and refined by Least Squares using version 2018/3 of ShelXL 2018/3 (Sheldrick, 2015). All non-hydrogen atoms were refined anisotropically. Hydrogen atom positions were calculated geometrically and refined using the riding model. Hydrogen atom positions were calculated geometrically and refined using the riding model.

_exptl_absorpt_process_details: CrysAlisPro 1.171.43.127a (Rigaku Oxford Diffraction, 2024) Numerical absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Table 1: Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for **03612**. *U*_{eq} is defined as 1/3 of the trace of the orthogonalised *U*_{ij}.

Atom	x	y	z	<i>U</i> _{eq}
Ru1	7259.1(2)	6303.2(2)	6357.2(2)	19.40(7)
Cl1	6926.5(7)	5642.4(4)	4090.9(6)	29.74(15)
Cl2	9336.6(6)	6795.1(4)	5949.9(7)	29.69(15)
N1	8327(2)	5254.5(13)	7251(2)	23.5(4)
C1	5429(2)	6037.2(17)	7030(3)	23.1(5)
C2	6550(3)	6166.1(16)	8199(3)	24.2(5)
C3	7261(3)	6918.8(17)	8325(3)	25.7(6)
C4	6939(3)	7492.0(16)	7216(3)	26.9(6)
C5	5878(3)	7353.0(16)	6027(3)	25.4(5)
C6	5100(2)	6634.9(17)	5946(3)	23.9(5)
C7	7140(3)	5454.9(17)	9077(3)	25.7(6)
C8	6862(3)	5227.9(19)	10350(3)	34.4(6)

Atom	x	y	z	U_{eq}
C9	7518(3)	4547(2)	11083(3)	40.6(7)
C10	8407(3)	4104.5(19)	10567(3)	37.1(7)
C11	8719(3)	4316.0(16)	9259(3)	29.0(6)
C12	9638(3)	3895.8(17)	8641(3)	33.5(7)
C13	9879(3)	4158.1(19)	7388(3)	36.2(7)
C14	9205(3)	4850.2(17)	6726(3)	29.9(6)
C15	8071(2)	5001.5(16)	8531(3)	23.2(5)
C16	3899(3)	6483.9(18)	4741(3)	29.1(6)
C17	2685(3)	6808(2)	5240(3)	40.7(7)
C18	3980(3)	6877(2)	3349(3)	43.4(8)

Table 2: Anisotropic Displacement Parameters ($\times 10^4$) **03612**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \dots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ru1	18.90(11)	18.34(11)	20.48(11)	-0.67(7)	3.51(7)	-1.04(7)
Cl1	36.4(3)	29.9(3)	23.3(3)	-4.4(3)	7.6(3)	-4.7(3)
Cl2	23.1(3)	27.5(3)	39.5(3)	3.4(3)	9.2(3)	-4.3(2)
N1	23.6(10)	20.7(11)	25.4(10)	-1.0(9)	3.8(9)	-0.5(9)
C1	21.1(12)	27.0(13)	22.3(12)	-1.9(11)	7.2(10)	-2.2(10)
C2	24.7(12)	28.8(14)	20.1(12)	-3.1(11)	7.1(10)	2.5(11)
C3	24.7(13)	27.1(14)	23.3(12)	-7.7(11)	1.7(10)	2.6(11)
C4	25.9(13)	19.5(13)	35.7(14)	-7.6(11)	7.8(11)	0.7(10)
C5	24.0(13)	23.1(13)	28.5(13)	1.0(11)	4.6(10)	5.1(10)
C6	17.9(12)	27.3(14)	26.4(13)	0.8(11)	4.6(10)	4.7(10)
C7	27.2(13)	27.6(14)	20.7(12)	-1.9(11)	2.4(10)	-3.4(11)
C8	39.3(16)	39.1(17)	25.4(13)	-1.6(12)	8.3(12)	-1.3(13)
C9	55(2)	42.5(18)	23.3(14)	6.2(13)	7.1(13)	-5.8(15)
C10	47.1(18)	28.1(15)	28.7(14)	6.6(12)	-6.5(13)	-2.2(13)
C11	31.3(14)	21.9(13)	28.4(13)	-0.1(11)	-4.3(11)	-5.7(11)
C12	30.0(14)	20.8(14)	41.8(16)	-0.4(12)	-8.4(12)	3.9(11)
C13	29.4(14)	31.1(15)	46.3(17)	-5.5(14)	4.7(13)	7.5(12)
C14	27.7(13)	27.5(15)	35.6(14)	-2.7(12)	9.8(11)	3.8(11)
C15	21.9(12)	22.2(13)	22.8(12)	-1.1(10)	-0.7(10)	-5.4(10)
C16	24.8(13)	30.2(15)	29.3(14)	2.9(11)	-0.1(11)	-4.6(11)
C17	23.5(14)	53(2)	41.5(17)	-1.5(15)	-1.0(12)	1.5(14)
C18	36.7(16)	57(2)	30.9(15)	9.2(15)	-3.5(13)	-8.6(15)

Table 3: Bond Lengths in Å for **03612**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	Cl1	2.4033(6)	C4	C5	1.416(4)
Ru1	Cl2	2.4066(6)	C5	C6	1.418(4)
Ru1	N1	2.119(2)	C6	C16	1.518(4)
Ru1	C1	2.179(3)	C7	C8	1.380(4)
Ru1	C2	2.090(3)	C7	C15	1.411(4)
Ru1	C3	2.158(3)	C8	C9	1.411(5)
Ru1	C4	2.176(3)	C9	C10	1.352(5)
Ru1	C5	2.213(3)	C10	C11	1.421(4)
Ru1	C6	2.240(2)	C11	C12	1.412(4)
N1	C14	1.316(4)	C11	C15	1.412(4)
N1	C15	1.389(3)	C12	C13	1.364(5)
C1	C2	1.438(4)	C13	C14	1.408(4)
C1	C6	1.421(4)	C16	C17	1.538(4)
C2	C3	1.428(4)	C16	C18	1.514(4)
C2	C7	1.491(4)			
C3	C4	1.410(4)			

Table 4: Bond Angles in ° for **03612**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl1	Ru1	Cl2	87.04(2)	C6	C1	C2	119.6(2)
N1	Ru1	Cl1	87.71(6)	C1	C2	Ru1	73.67(14)
N1	Ru1	Cl2	86.55(6)	C1	C2	C7	119.0(2)
N1	Ru1	C1	96.91(9)	C3	C2	Ru1	72.97(15)
N1	Ru1	C3	97.06(9)	C3	C2	C1	120.0(2)
N1	Ru1	C4	132.98(9)	C3	C2	C7	119.6(2)
N1	Ru1	C5	161.67(9)	C7	C2	Ru1	113.29(17)
N1	Ru1	C6	132.34(9)	C2	C3	Ru1	67.79(14)
C1	Ru1	Cl1	103.32(7)	C4	C3	Ru1	71.68(15)
C1	Ru1	Cl2	169.16(7)	C4	C3	C2	119.0(2)
C1	Ru1	C5	67.98(10)	C3	C4	Ru1	70.35(15)
C1	Ru1	C6	37.48(10)	C3	C4	C5	121.2(3)
C2	Ru1	Cl1	136.66(8)	C5	C4	Ru1	72.60(15)
C2	Ru1	Cl2	132.44(7)	C4	C5	Ru1	69.77(15)
C2	Ru1	N1	79.28(9)	C4	C5	C6	120.1(2)
C2	Ru1	C1	39.32(10)	C6	C5	Ru1	72.49(15)
C2	Ru1	C3	39.23(10)	C1	C6	Ru1	68.91(14)
C2	Ru1	C4	69.91(11)	C1	C6	C16	118.2(2)
C2	Ru1	C5	82.40(10)	C5	C6	Ru1	70.38(14)
C2	Ru1	C6	69.52(10)	C5	C6	C1	119.7(2)
C3	Ru1	Cl1	172.02(7)	C5	C6	C16	122.1(2)
C3	Ru1	Cl2	99.59(7)	C16	C6	Ru1	134.61(19)
C3	Ru1	C1	69.84(10)	C8	C7	C2	125.5(3)
C3	Ru1	C4	37.98(11)	C8	C7	C15	119.4(3)
C3	Ru1	C5	68.54(10)	C15	C7	C2	115.0(2)
C3	Ru1	C6	81.02(10)	C7	C8	C9	119.3(3)
C4	Ru1	Cl1	138.75(8)	C10	C9	C8	121.8(3)
C4	Ru1	Cl2	88.90(8)	C9	C10	C11	120.6(3)
C4	Ru1	C1	81.22(10)	C12	C11	C10	124.7(3)
C4	Ru1	C5	37.63(10)	C12	C11	C15	117.7(3)
C4	Ru1	C6	67.57(10)	C15	C11	C10	117.5(3)
C5	Ru1	Cl1	105.43(7)	C13	C12	C11	120.0(3)
C5	Ru1	Cl2	106.50(7)	C12	C13	C14	119.3(3)
C5	Ru1	C6	37.14(10)	N1	C14	C13	122.9(3)
C6	Ru1	Cl1	91.04(7)	N1	C15	C7	117.5(2)
C6	Ru1	Cl2	140.99(7)	N1	C15	C11	121.3(2)
C14	N1	Ru1	126.22(19)	C7	C15	C11	121.2(2)
C14	N1	C15	118.9(2)	C6	C16	C17	106.4(2)
C15	N1	Ru1	114.90(17)	C18	C16	C6	114.5(2)
C2	C1	Ru1	67.01(14)	C18	C16	C17	110.4(3)
C6	C1	Ru1	73.61(15)				

Table 5: Torsion Angles in ° for **03612**.

Atom	Atom	Atom	Atom	Angle/°
Ru1	N1	C14	C13	179.7(2)
Ru1	N1	C15	C7	0.6(3)
Ru1	N1	C15	C11	-179.41(18)
Ru1	C1	C2	C3	58.5(2)
Ru1	C1	C2	C7	-108.0(2)
Ru1	C1	C6	C5	-50.6(2)
Ru1	C1	C6	C16	130.3(2)
Ru1	C2	C3	C4	52.1(2)
Ru1	C2	C7	C8	179.2(2)
Ru1	C2	C7	C15	0.3(3)
Ru1	C3	C4	C5	54.1(2)
Ru1	C4	C5	C6	54.2(2)
Ru1	C5	C6	C1	50.0(2)
Ru1	C5	C6	C16	-131.0(2)
Ru1	C6	C16	C17	173.9(2)
Ru1	C6	C16	C18	-64.0(4)
C1	C2	C3	Ru1	-58.9(2)

Atom	Atom	Atom	Atom	Angle/°
C1	C2	C3	C4	-6.8(4)
C1	C2	C7	C8	-97.1(3)
C1	C2	C7	C15	84.0(3)
C1	C6	C16	C17	86.4(3)
C1	C6	C16	C18	-151.4(3)
C2	C1	C6	Ru1	50.5(2)
C2	C1	C6	C5	-0.1(4)
C2	C1	C6	C16	-179.1(2)
C2	C3	C4	Ru1	-50.3(2)
C2	C3	C4	C5	3.7(4)
C2	C7	C8	C9	-178.7(3)
C2	C7	C15	N1	-0.6(3)
C2	C7	C15	C11	179.4(2)
C3	C2	C7	C8	96.3(3)
C3	C2	C7	C15	-82.6(3)
C3	C4	C5	Ru1	-53.0(2)
C3	C4	C5	C6	1.2(4)
C4	C5	C6	Ru1	-52.9(2)
C4	C5	C6	C1	-3.0(4)
C4	C5	C6	C16	176.0(2)
C5	C6	C16	C17	-92.6(3)
C5	C6	C16	C18	29.6(4)
C6	C1	C2	Ru1	-53.5(2)
C6	C1	C2	C3	5.0(4)
C6	C1	C2	C7	-161.5(2)
C7	C2	C3	Ru1	107.6(2)
C7	C2	C3	C4	159.7(2)
C7	C8	C9	C10	-0.6(5)
C8	C7	C15	N1	-179.6(2)
C8	C7	C15	C11	0.4(4)
C8	C9	C10	C11	0.4(5)
C9	C10	C11	C12	179.5(3)
C9	C10	C11	C15	0.2(4)
C10	C11	C12	C13	-179.0(3)
C10	C11	C15	N1	179.4(2)
C10	C11	C15	C7	-0.6(4)
C11	C12	C13	C14	0.1(4)
C12	C11	C15	N1	0.1(4)
C12	C11	C15	C7	-180.0(2)
C12	C13	C14	N1	-1.1(4)
C14	N1	C15	C7	179.1(2)
C14	N1	C15	C11	-1.0(4)
C15	N1	C14	C13	1.5(4)
C15	C7	C8	C9	0.1(4)
C15	C11	C12	C13	0.3(4)

Table 6: Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **03612**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} .

Atom	x	y	z	U_{eq}
H1	4911.44	5555.07	6983.65	28
H3	7940.68	7031.77	9144.32	31
H4	7442.95	7979.94	7267.28	32
H5	5686.26	7741.62	5281.93	30
H8	6235.69	5526.82	10729.39	41
H9	7330.54	4395.65	11962.96	49
H10	8827.27	3647.58	11084.55	44
H12	10088.88	3430.2	9098.73	40
H13	10495.7	3877.02	6967.17	43
H14	9391.79	5033.11	5861.86	36
H16	3792.07	5882.55	4589.97	35
H17A	2608.86	6521.41	6105.55	61

Atom	x	y	z	U_{eq}
H17B	1877.38	6715.98	4498.95	61
H17C	2793.72	7392.99	5435.13	61
H18A	4009.01	7470.79	3459.24	65
H18B	3196.94	6723.97	2615.39	65
H18C	4786.88	6690.54	3073.32	65

Citations

O.V. Dolomanov and L.J. Bourhis and R.J. Gildea and J.A.K. Howard and H. Puschmann, Olex2: A complete structure solution, refinement and analysis program, *J. Appl. Cryst.*, (2009), **42**, 339-341.