Table 1. Crystal data and structure refinement for **2**.

Empirical formula	$C_{29}H_{47}ClN_2Ru$
Formula weight	560.21
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 9.1472(8) Å α = 90 deg b = 14.2579(11) Å β = 90 deg c = 21.9374(19) Å γ = 90 deg
Volume	2861.1(4) $Å^3$
Z, Calculated density	4, 1.301 g/cm^3
Absorption coefficient	0.660 mm^{-1}
F(000)	1184
Crystal size	0.50 x 0.50 x 0.34 mm
Theta range for data collection	1.70 to 36.37 deg.
Limiting indices	-15≤h≤14, -22≤k≤22, -35≤l≤29
Reflections collected / unique	70034 / 13262 [R(int) = 0.0569]
Completeness to theta = 36.37	97.2 %
Absorption correction	Empirical
Max. and min. transmission	1.0000 and 0.7732
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13262 / 0 / 485
Goodness-of-fit on F^2	0.781
Final R indices [I>2sigma(I)]	R1 = 0.0256, wR2 = 0.0468
R indices (all data)	R1 = 0.0461, wR2 = 0.0479
Absolute structure parameter	-0.052(14)
Largest diff. peak and hole	0.488 and -0.637 $e.A^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	7479(1)	3650(1)	7978(1)	19(1)
Cl(1)	10052(1)	3789(1)	8100(1)	29(1)
N(1)	8384(1)	1568(1)	8206(1)	22(1)
C(1)	6456(2)	4873(1)	7616(1)	29(1)
N(2)	7804(1)	1756(1)	7270(1)	21(1)
C(2)	6873(2)	5069(1)	8228(1)	27(1)
C(3)	6165(2)	4391(1)	8606(1)	27(1)
C(4)	5226(2)	3818(1)	8238(1)	27(1)
C(5)	5414(2)	4118(1)	7615(1)	29(1)
C(6)	6990(3)	5397(2)	7063(1)	47(1)
C(7)	7900(2)	5818(2)	8434(1)	41(1)
C(8)	6296(3)	4332(2)	9286(1)	42(1)
C(9)	4145(2)	3098(2)	8443(1)	43(1)
C(10)	4505(2)	3786(2)	7092(1)	47(1)
C(11)	7718(3)	1349(2)	9924(1)	49(1)
C(12)	6885(3)	611(2)	10325(1)	58(1)
C(13)	5349(3)	513(2)	10119(1)	63(1)
C(14)	5331(3)	217(3)	9443(1)	74(1)
C(15)	6148(3)	940(2)	9047(1)	53(1)
C(16)	7707(2)	1052(1)	9252(1)	33(1)
C(17)	8610(2)	1736(1)	8864(1)	26(1)
C(18)	10241(2)	1683(2)	9011(1)	40(1)
C(19)	7829(1)	2218(1)	7816(1)	20(1)
C(20)	8702(2)	738(1)	7909(1)	27(1)
C(21)	8347(2)	854(1)	7325(1)	26(1)
C(22)	5978(2)	1551(2)	6474(1)	36(1)
C(23)	7230(2)	2160(1)	6699(1)	24(1)
C(24)	8435(2)	2333(1)	6227(1)	24(1)
C(25)	9652(2)	2951(1)	6482(1)	26(1)
C(26)	10793(2)	3209(1)	6005(1)	33(1)
C(27)	10111(2)	3665(1)	5449(1)	35(1)
C(28)	8941(2)	3030(2)	5178(1)	40(1)
C(29)	7790(2)	2775(2)	5654(1)	34(1)

Table 3. Bond lengths [Å] and angles [deg] for **2**.

Ru(1)-C(19)	2.0966(15)
Ru(1)-C(3)	2.1120(16)
Ru(1)-C(1)	2.1318(16)
Ru(1)-C(4)	2.1518(18)
Ru(1)-C(5)	2.1558(16)
Ru(1)-C(2)	2.1677(15)
Ru(1)-Cl(1)	2.3766(5)
N(1)-C(19)	1.3592(18)
N(1)-C(20)	1.382(2)
N(1)-C(17)	1.477(2)
C(1)-C(2)	1.422(2)
C(1)-C(5)	1.437(2)
C(1)-C(6)	1.506(3)
N(2)-C(19)	1.3682(18)
N(2)-C(21)	1.385(2)
N(2)-C(23)	1.476(2)
C(2)-C(3)	1.430(2)
C(2)-C(7)	1.493(2)
C(3)-C(4)	1.434(2)
C(3)-C(8)	1.498(3)
C(4)-C(5)	1.443(3)
C(4)-C(9)	1.494(3)
C(5)-C(10)	1.494(3)
C(11)-C(16)	1.534(2)
C(11)-C(12)	1.568(3)
C(12)-C(13)	1.483(3)
C(13)-C(14)	1.542(3)
C(14)-C(15)	1.541(3)
C(15)-C(16)	1.504(3)
C(16)-C(17)	1.536(2)
C(17)-C(18)	1.529(3)
C(20)-C(21)	1.333(2)
C(22)-C(23)	1.520(2)
C(23)-C(24)	1.531(2)
C(24)-C(25)	1.526(2)
C(24)-C(29)	1.526(2)
C(25)-C(26)	1.523(2)
C(26)-C(27)	1.515(3)
C(27)-C(28)	1.523(3)
C(28)-C(29)	1.527(3)
C(19)-Ru(1)-C(3)	133.16(6)
C(19)-Ru(1)-C(1)	143.17(6)
C(3)-Ru(1)-C(1)	65.43(7)
C(19)-Ru(1)-C(4)	107.43(6)
C(3)-Ru(1)-C(4)	39.29(7)
C(1)-Ru(1)-C(4)	65.62(7)
C(19)-Ru(1)-C(5)	111.88(6)
C(3)-Ru(1)-C(5)	65.66(7)
C(1)-Ru(1)-C(5)	39.16(6)

C(4)-Ru(1)-C(5)	39.15(7)
C(19)-Ru(1)-C(2)	172.04(6)
C(3)-Ru(1)-C(2)	39.01(6)
C(1)-Ru(1)-C(2)	38.61(6)
C(4)-Ru(1)-C(2)	65.42(7)
C(5)-Ru(1)-C(2)	65.19(6)
C(19)-Ru(1)-Cl(1)	87.08(4)
C(3)-Ru(1)-Cl(1)	116.64(5)
C(1)-Ru(1)-Cl(1)	114.10(5)
C(4)-Ru(1)-Cl(1)	155.39(5)
C(5)-Ru(1)-Cl(1)	152.03(5)
C(2)-Ru(1)-Cl(1)	98.45(4)
C(19)-N(1)-C(20)	111.46(13)
C(19)-N(1)-C(17)	123.81(13)
C(20)-N(1)-C(17)	124.72(13)
C(2)-C(1)-C(5)	109.11(15)
C(2)-C(1)-C(6)	125.10(18)
C(5)-C(1)-C(6)	125.77(19)
C(2)-C(1)-Ru(1)	72.06(10)
C(5)-C(1)-Ru(1)	71.32(9)
C(6)-C(1)-Ru(1)	124.26(13)
C(19)-N(2)-C(21)	111.42(13)
C(19)-N(2)-C(23)	124.18(12)
C(21)-N(2)-C(23)	124.37(13)
C(1)-C(2)-C(3)	107.07(14)
C(1)-C(2)-C(7)	126.51(18)
C(3)-C(2)-C(7)	126.38(19)
C(1)-C(2)-Ru(1)	69.33(9)
C(3)-C(2)-Ru(1)	68.39(9)
C(7)-C(2)-Ru(1)	125.71(12)
C(2)-C(3)-C(4)	109.20(16)
C(2)-C(3)-C(8)	125.44(17)
C(4)-C(3)-C(8)	125.22(18)
C(2)-C(3)-Ru(1)	72.60(9)
C(4)-C(3)-Ru(1)	71.85(10)
C(8)-C(3)-Ru(1)	125.19(14)
C(3)-C(4)-C(5)	107.08(16)
C(3)-C(4)-C(9)	128.2(2)
C(5)-C(4)-C(9)	124.56(18)
C(3)-C(4)-Ru(1)	68.86(9)
C(5)-C(4)-Ru(1)	70.57(10)
C(9)-C(4)-Ru(1)	129.58(14)
C(1)-C(5)-C(4)	107.38(15)
C(1)-C(5)-C(10)	127.46(19)
C(4)-C(5)-C(10)	124.56(18)
C(1)-C(5)-Ru(1)	69.52(9)
C(4)-C(5)-Ru(1)	70.27(10)
C(10)-C(5)-Ru(1)	132.35(13)
C(16)-C(11)-C(12)	110.54(19)
C(13)-C(12)-C(11)	110.7(2)
C(12)-C(13)-C(14)	109.2(2)
C(15)-C(14)-C(13)	110.7(2)
C(16)-C(15)-C(14)	111.2(2)
C(15)-C(16)-C(11)	108.86(17)

C(15)-C(16)-C(17)	114.27(15)
C(11)-C(16)-C(17)	110.78(16)
N(1)-C(17)-C(18)	109.62(15)
N(1)-C(17)-C(16)	111.35(13)
C(18)-C(17)-C(16)	112.07(15)
N(1)-C(19)-N(2)	103.26(12)
N(1)-C(19)-Ru(1)	127.90(11)
N(2)-C(19)-Ru(1)	127.93(11)
C(21)-C(20)-N(1)	107.22(14)
C(20)-C(21)-N(2)	106.63(15)
N(2)-C(23)-C(22)	108.65(14)
N(2)-C(23)-C(24)	112.34(13)
C(22)-C(23)-C(24)	114.56(14)
C(25)-C(24)-C(29)	110.16(14)
C(25)-C(24)-C(23)	111.79(13)
C(29)-C(24)-C(23)	110.17(14)
C(26)-C(25)-C(24)	112.83(15)
C(27)-C(26)-C(25)	111.94(15)
C(26)-C(27)-C(28)	110.42(16)
C(27)-C(28)-C(29)	111.00(16)
C(24)-C(29)-C(28)	113.31(16)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **2**. The anisotropic displacement factor exponent takes the form: $-2\ pi^2\ [\ h^2\ a^{*2}\ U11 + ... + 2\ h\ k\ a^*\ b^*\ U12\ ]$

	U11	U22	U33	U23	U13	U12
Ru(1)	18(1)	15(1)	24(1)	-1(1)	-1(1)	1(1)
Cl(1)	21(1)	22(1)	45(1)	2(1)	-5(1)	-2(1)
N(1)	26(1)	18(1)	22(1)	1(1)	3(1)	2(1)
C(1)	30(1)	21(1)	35(1)	5(1)	-2(1)	8(1)
N(2)	23(1)	19(1)	21(1)	-3(1)	5(1)	-1(1)
C(2)	23(1)	17(1)	41(1)	-6(1)	1(1)	4(1)
C(3)	21(1)	28(1)	31(1)	-6(1)	1(1)	4(1)
C(4)	18(1)	22(1)	42(1)	-4(1)	0(1)	2(1)
C(5)	28(1)	24(1)	34(1)	-5(1)	-7(1)	8(1)
C(6)	56(1)	43(1)	44(1)	18(1)	-1(1)	12(1)
C(7)	29(1)	25(1)	69(2)	-11(1)	0(1)	-3(1)
C(8)	37(1)	58(2)	31(1)	-6(1)	4(1)	4(1)
C(9)	23(1)	35(1)	72(2)	-3(1)	8(1)	-5(1)
C(10)	36(1)	56(2)	48(2)	-18(1)	-20(1)	19(1)
C(11)	46(2)	77(1)	23(1)	-5(1)	-3(1)	-9(1)
C(12)	48(1)	104(2)	24(1)	8(1)	3(1)	0(1)
C(13)	56(2)	100(2)	32(1)	4(1)	15(1)	-23(1)
C(14)	68(2)	120(3)	34(1)	5(1)	5(1)	-53(2)
C(15)	43(1)	85(2)	30(1)	2(1)	-1(1)	-18(1)
C(16)	38(1)	37(1)	23(1)	-1(1)	1(1)	3(1)
C(17)	32(1)	21(1)	23(1)	1(1)	-3(1)	4(1)
C(18)	34(1)	50(1)	36(1)	12(1)	-7(1)	1(1)
C(19)	17(1)	23(1)	20(1)	2(1)	4(1)	-2(1)
C(20)	31(1)	17(1)	32(1)	0(1)	7(1)	3(1)
C(21)	34(1)	15(1)	30(1)	-2(1)	9(1)	0(1)
C(22)	34(1)	42(1)	33(1)	-3(1)	0(1)	-14(1)
C(23)	25(1)	26(1)	22(1)	-2(1)	2(1)	-1(1)
C(24)	28(1)	23(1)	21(1)	-2(1)	5(1)	0(1)
C(25)	24(1)	30(1)	24(1)	4(1)	0(1)	-2(1)
C(26)	29(1)	36(1)	34(1)	9(1)	4(1)	-3(1)
C(27)	41(1)	35(1)	28(1)	5(1)	8(1)	-6(1)
C(28)	48(1)	50(1)	23(1)	4(1)	3(1)	-7(1)
C(29)	38(1)	42(1)	21(1)	1(1)	-3(1)	-4(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **2**.

	x	y	z	U(eq)
H(6B)	6290(20)	5811(15)	7000(9)	42(5)
H(6A)	6947(18)	5011(13)	6733(9)	30(5)
H(6C)	8010(30)	5790(20)	7157(13)	99(11)
H(7C)	8550(20)	6012(15)	8133(10)	49(6)
H(7B)	7420(40)	6433(19)	8477(12)	102(9)
H(7A)	8430(30)	5689(19)	8670(12)	71(10)
H(7B)	7250(30)	4573(14)	9418(9)	61(7)
H(8A)	5600(20)	4691(14)	9491(8)	28(5)
H(8C)	6120(30)	3827(18)	9452(12)	78(10)
H(9C)	4230(20)	2490(15)	8135(10)	56(6)
H(9B)	4340(20)	2956(16)	8852(11)	52(7)
H(9A)	3180(30)	3258(16)	8419(10)	61(7)
H(10A)	3680(30)	4161(17)	7175(11)	71(8)
H(10B)	4230(20)	3162(14)	7149(8)	35(6)
H(10C)	4900(30)	3872(18)	6740(12)	81(10)
H(11A)	7260(20)	1978(12)	9940(8)	35(5)
H(11B)	8750(20)	1424(15)	10081(9)	49(6)
H(12A)	7520(30)	-152(17)	10302(10)	83(7)
H(12B)	6790(30)	971(19)	10812(13)	99(9)
H(13A)	5290(30)	1295(18)	10191(10)	63(7)
H(13B)	4800(20)	-9(15)	10335(10)	52(7)
H(14A)	4410(30)	166(16)	9318(11)	62(8)
H(14B)	6040(20)	-428(15)	9439(9)	41(6)
H(15B)	6280(30)	530(20)	8550(15)	111(11)
H(15B)	5740(30)	1589(18)	9086(12)	72(9)
H(16)	7891(19)	294(13)	9198(8)	42
H(17)	8318(16)	2333(11)	8933(7)	15(4)
H(18A)	10860(20)	2134(14)	8737(9)	38(5)
H(18B)	10390(30)	1817(16)	9457(12)	68(8)
H(18C)	10620(20)	963(16)	8941(9)	53(6)
H(20)	9176(19)	180(13)	8110(8)	34(5)
H(21)	8443(18)	434(12)	7022(8)	23(4)
H(22A)	5490(20)	1838(13)	6174(9)	38(6)
H(22B)	5335(19)	1414(12)	6799(8)	28(4)
H(22C)	6300(20)	1032(16)	6364(10)	48(7)
H(23)	6799(19)	2777(13)	6833(8)	39(5)
H(24)	8830(20)	1768(13)	6137(8)	24(5)
H(25B)	10111(16)	2674(10)	6797(7)	12(4)
H(25A)	9235(17)	3543(12)	6629(7)	19(4)
H(26B)	11540(20)	3634(14)	6188(9)	45(6)
H(26A)	11320(20)	2681(13)	5869(8)	31(5)
H(27B)	9690(20)	4295(15)	5598(9)	51(6)
H(27A)	10850(20)	3808(13)	5157(8)	34(5)
H(28B)	8430(20)	3288(14)	4850(10)	45(6)
H(28A)	9397(19)	2435(14)	5034(8)	33(5)
H(29A)	7080(20)	2324(14)	5467(9)	45(6)
H(29B)	7370(20)	3183(12)	5756(8)	23(5)

Table 6. Crystal data and structure refinement for **3**.

Empirical formula	$C_{33}H_{51}ClN_2Ru$
Formula weight	612.28
Temperature	150(2) K
Wavelength	0.71073
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 8.9976(4) α = 90.000(10) deg.
	b = 15.3812(7) β = 95.806(10) deg.
	c = 11.3825(5) γ = 90.000(10) deg.
Volume	1567.19(12) ^{3}
Z, Calculated density	2, 1.297 Mg/cm^3
Absorption coefficient	0.609 mm^{-1}
F(000)	648
Crystal size	0.45 x 0.28 x 0.18 mm
Theta range for data collection	1.80 to 35.82 deg.
Limiting indices	-13<=h<=14, -23<=k<=25, -10<=l<=18
Reflections collected / unique	18433 / 11915 [R(int) = 0.0273]
Completeness to theta = 35.82	89.2 %
Absorption correction	Empirical
Max. and min. transmission	1.0000 and 0.8069
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11915 / 1 / 417
Goodness-of-fit on F^2	0.714
Final R indices [I>2sigma(I)]	R1 = 0.0282, wR2 = 0.0563
R indices (all data)	R1 = 0.0513, wR2 = 0.0689
Absolute structure parameter	0.001(17)
Largest diff. peak and hole	1.550 and -0.600 e.A^{-3}

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3** U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	258(1)	0(1)	-2201(1)	18(1)
C(1)	1270(2)	-338(1)	-3777(2)	20(1)
N(1)	1977(3)	1599(1)	-961(2)	20(1)
Cl(1)	-1750(1)	87(1)	-1008(1)	33(1)
N(2)	111(2)	2028(1)	-2145(2)	22(1)
C(2)	-216(2)	-709(1)	-3801(2)	21(1)
C(3)	-230(3)	-1307(1)	-2849(2)	23(1)
C(4)	1194(3)	-1269(2)	-2192(2)	25(1)
C(5)	2135(2)	-684(1)	-2778(2)	22(1)
C(6)	1845(3)	218(1)	-4707(2)	29(1)
C(7)	-1469(3)	-557(2)	-4731(2)	29(1)
C(8)	-1539(3)	-1834(2)	-2552(3)	34(1)
C(9)	1671(4)	-1786(2)	-1090(3)	35(1)
C(10)	3802(2)	-565(2)	-2520(2)	32(1)
C(11)	6706(3)	295(2)	2458(2)	43(1)
C(12)	5090(3)	-427(2)	882(2)	31(1)
C(13)	5421(3)	439(2)	1479(2)	28(1)
C(14)	4151(3)	1012(2)	1926(2)	28(1)
C(15)	5095(3)	1813(2)	1668(2)	34(1)
C(16)	5737(2)	1246(2)	718(2)	26(1)
C(17)	4681(2)	1289(2)	-423(2)	23(1)
C(18)	3051(2)	1047(2)	-236(2)	20(1)
C(19)	2707(2)	1046(2)	1077(2)	25(1)
C(20)	1570(3)	344(2)	1311(2)	34(1)
C(21)	870(2)	1295(2)	-1763(2)	17(1)
C(22)	1919(3)	2496(2)	-870(2)	27(1)
C(23)	754(3)	2766(2)	-1611(2)	28(1)
C(24)	-533(3)	2102(2)	-4985(2)	33(1)
C(25)	-1254(3)	2583(2)	-4026(2)	23(1)
C(26)	-1303(3)	2018(2)	-2915(2)	21(1)
C(27)	-2631(3)	2213(2)	-2195(2)	28(1)
C(28)	-3932(3)	2652(2)	-2946(2)	27(1)
C(29)	-3346(3)	3499(2)	-3452(3)	32(1)
C(30)	-2825(3)	2924(2)	-4440(2)	25(1)
C(31)	-4143(3)	2293(2)	-4222(2)	28(1)
C(32)	-4056(3)	1318(2)	-4421(2)	35(1)
C(33)	-5598(3)	2613(2)	-4898(3)	46(1)

Table 8. Bond lengths [ ] and angles [deg] for **3**.

Ru(1)-C(21)	2.113(2)
Ru(1)-C(4)	2.125(3)
Ru(1)-C(2)	2.128(2)
Ru(1)-C(5)	2.148(2)
Ru(1)-C(1)	2.155(2)
Ru(1)-C(3)	2.170(2)
Ru(1)-Cl(1)	2.3711(5)
C(1)-C(5)	1.415(3)
C(1)-C(2)	1.452(3)
C(1)-C(6)	1.494(3)
N(1)-C(21)	1.363(3)
N(1)-C(22)	1.386(3)
N(1)-C(18)	1.474(3)
N(2)-C(21)	1.367(3)
N(2)-C(23)	1.387(3)
N(2)-C(26)	1.470(3)
C(2)-C(3)	1.423(3)
C(2)-C(7)	1.484(3)
C(3)-C(4)	1.418(3)
C(3)-C(8)	1.496(4)
C(4)-C(5)	1.443(4)
C(4)-C(9)	1.511(4)
C(5)-C(10)	1.510(3)
C(11)-C(13)	1.538(3)
C(12)-C(13)	1.512(3)
C(13)-C(16)	1.556(4)
C(13)-C(14)	1.569(3)
C(14)-C(19)	1.540(3)
C(14)-C(15)	1.542(4)
C(15)-C(16)	1.546(4)
C(16)-C(17)	1.531(3)
C(17)-C(18)	1.548(3)
C(18)-C(19)	1.556(3)
C(19)-C(20)	1.529(3)
C(22)-C(23)	1.344(3)
C(24)-C(25)	1.517(4)
C(25)-C(30)	1.536(3)
C(25)-C(26)	1.539(3)
C(26)-C(27)	1.545(4)
C(27)-C(28)	1.534(3)
C(28)-C(29)	1.539(4)
C(28)-C(31)	1.547(4)
C(29)-C(30)	1.540(4)
C(30)-C(31)	1.572(3)
C(31)-C(32)	1.520(4)
C(31)-C(33)	1.531(3)
C(21)-Ru(1)-C(4)	140.42(8)
C(21)-Ru(1)-C(2)	135.22(9)
C(4)-Ru(1)-C(2)	65.09(9)
C(21)-Ru(1)-C(5)	109.86(8)
C(4)-Ru(1)-C(5)	39.47(10)

C(2)-Ru(1)-C(5)	65.38(8)
C(21)-Ru(1)-C(1)	107.56(8)
C(4)-Ru(1)-C(1)	65.28(9)
C(2)-Ru(1)-C(1)	39.61(8)
C(5)-Ru(1)-C(1)	38.39(8)
C(21)-Ru(1)-C(3)	172.83(10)
C(4)-Ru(1)-C(3)	38.53(9)
C(2)-Ru(1)-C(3)	38.64(9)
C(5)-Ru(1)-C(3)	65.21(9)
C(1)-Ru(1)-C(3)	65.29(8)
C(21)-Ru(1)-Cl(1)	90.39(7)
C(4)-Ru(1)-Cl(1)	111.95(8)
C(2)-Ru(1)-Cl(1)	114.89(6)
C(5)-Ru(1)-Cl(1)	150.54(7)
C(1)-Ru(1)-Cl(1)	154.27(6)
C(3)-Ru(1)-Cl(1)	96.17(7)
C(5)-C(1)-C(2)	107.36(19)
C(5)-C(1)-C(6)	125.7(2)
C(2)-C(1)-C(6)	126.5(2)
C(5)-C(1)-Ru(1)	70.54(13)
C(2)-C(1)-Ru(1)	69.18(12)
C(6)-C(1)-Ru(1)	131.14(15)
C(21)-N(1)-C(22)	111.2(2)
C(21)-N(1)-C(18)	124.8(2)
C(22)-N(1)-C(18)	123.9(2)
C(21)-N(2)-C(23)	111.29(18)
C(21)-N(2)-C(26)	123.74(19)
C(23)-N(2)-C(26)	124.59(19)
C(3)-C(2)-C(1)	108.54(19)
C(3)-C(2)-C(7)	125.4(2)
C(1)-C(2)-C(7)	125.7(2)
C(3)-C(2)-Ru(1)	72.27(12)
C(1)-C(2)-Ru(1)	71.21(12)
C(7)-C(2)-Ru(1)	126.98(16)
C(4)-C(3)-C(2)	107.3(2)
C(4)-C(3)-C(8)	126.4(2)
C(2)-C(3)-C(8)	126.2(2)
C(4)-C(3)-Ru(1)	69.04(14)
C(2)-C(3)-Ru(1)	69.09(12)
C(8)-C(3)-Ru(1)	124.19(18)
C(3)-C(4)-C(5)	108.8(2)
C(3)-C(4)-C(9)	125.6(2)
C(5)-C(4)-C(9)	125.5(2)
C(3)-C(4)-Ru(1)	72.43(13)
C(5)-C(4)-Ru(1)	71.12(14)
C(9)-C(4)-Ru(1)	124.49(19)
C(1)-C(5)-C(4)	107.76(19)
C(1)-C(5)-C(10)	124.4(2)
C(4)-C(5)-C(10)	127.1(2)
C(1)-C(5)-Ru(1)	71.07(12)
C(4)-C(5)-Ru(1)	69.41(13)
C(10)-C(5)-Ru(1)	132.62(16)
C(12)-C(13)-C(11)	107.3(2)
C(12)-C(13)-C(16)	119.43(19)

C(11)-C(13)-C(16)	110.6(2)
C(12)-C(13)-C(14)	121.7(2)
C(11)-C(13)-C(14)	111.4(2)
C(16)-C(13)-C(14)	84.94(18)
C(19)-C(14)-C(15)	107.4(2)
C(19)-C(14)-C(13)	114.26(19)
C(15)-C(14)-C(13)	87.34(19)
C(14)-C(15)-C(16)	86.24(19)
C(17)-C(16)-C(15)	109.0(2)
C(17)-C(16)-C(13)	111.97(18)
C(15)-C(16)-C(13)	87.67(19)
C(16)-C(17)-C(18)	112.83(19)
N(1)-C(18)-C(17)	111.13(19)
N(1)-C(18)-C(19)	110.87(18)
C(17)-C(18)-C(19)	114.54(17)
C(20)-C(19)-C(14)	113.8(2)
C(20)-C(19)-C(18)	111.70(19)
C(14)-C(19)-C(18)	111.48(18)
N(1)-C(21)-N(2)	103.8(2)
N(1)-C(21)-Ru(1)	129.53(17)
N(2)-C(21)-Ru(1)	126.34(15)
C(23)-C(22)-N(1)	107.1(2)
C(22)-C(23)-N(2)	106.6(2)
C(24)-C(25)-C(30)	113.2(2)
C(24)-C(25)-C(26)	111.4(2)
C(30)-C(25)-C(26)	110.04(19)
N(2)-C(26)-C(25)	112.87(19)
N(2)-C(26)-C(27)	110.5(2)
C(25)-C(26)-C(27)	114.4(2)
C(28)-C(27)-C(26)	112.2(2)
C(27)-C(28)-C(29)	108.0(2)
C(27)-C(28)-C(31)	112.3(2)
C(29)-C(28)-C(31)	88.01(19)
C(28)-C(29)-C(30)	85.90(19)
C(25)-C(30)-C(29)	108.1(2)
C(25)-C(30)-C(31)	115.22(18)
C(29)-C(30)-C(31)	87.09(19)
C(32)-C(31)-C(33)	107.3(2)
C(32)-C(31)-C(28)	119.3(2)
C(33)-C(31)-C(28)	112.0(2)
C(32)-C(31)-C(30)	122.4(2)
C(33)-C(31)-C(30)	110.0(2)
C(28)-C(31)-C(30)	84.53(18)

Table 9. Anisotropic displacement parameters ($A^2 \times 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Ru(1)	18(1)	16(1)	19(1)	-2(1)	3(1)	-1(1)
C(1)	23(1)	16(1)	21(1)	-5(1)	4(1)	0(1)
N(1)	22(1)	16(1)	22(1)	0(1)	-2(1)	0(1)
Cl(1)	30(1)	29(1)	44(1)	-3(1)	20(1)	-2(1)
N(2)	22(1)	17(1)	24(1)	2(1)	-1(1)	-1(1)
C(2)	25(1)	16(1)	21(1)	-3(1)	1(1)	-2(1)
C(3)	28(1)	18(1)	24(1)	-5(1)	4(1)	-3(1)
C(4)	33(1)	21(1)	22(1)	-1(1)	4(1)	6(1)
C(5)	23(1)	22(1)	22(1)	-7(1)	3(1)	1(1)
C(6)	32(1)	28(2)	29(1)	1(1)	11(1)	1(1)
C(7)	27(1)	29(1)	30(1)	-3(1)	-7(1)	-3(1)
C(8)	41(2)	23(1)	37(2)	-3(1)	8(1)	-12(1)
C(9)	43(2)	32(2)	31(2)	3(1)	2(1)	9(1)
C(10)	23(1)	43(2)	30(1)	-10(1)	1(1)	4(1)
C(11)	33(1)	61(2)	32(1)	7(1)	-10(1)	5(1)
C(12)	30(1)	32(1)	30(1)	8(1)	2(1)	6(1)
C(13)	22(1)	40(1)	20(1)	1(1)	-3(1)	2(1)
C(14)	27(1)	41(1)	17(1)	-3(1)	2(1)	-1(1)
C(15)	35(1)	36(2)	31(1)	-12(1)	0(1)	-2(1)
C(16)	20(1)	34(1)	25(1)	-5(1)	0(1)	-3(1)
C(17)	21(1)	28(1)	21(1)	0(1)	2(1)	-3(1)
C(18)	20(1)	20(1)	20(1)	0(1)	0(1)	1(1)
C(19)	23(1)	31(1)	21(1)	0(1)	3(1)	5(1)
C(20)	26(1)	48(2)	28(1)	9(1)	4(1)	-4(1)
C(21)	20(1)	18(1)	14(1)	2(1)	3(1)	0(1)
C(22)	31(1)	18(1)	32(1)	-3(1)	-3(1)	-3(1)
C(23)	32(1)	16(1)	35(1)	2(1)	-4(1)	-2(1)
C(24)	39(1)	31(1)	30(1)	10(1)	12(1)	10(1)
C(25)	25(1)	21(1)	24(1)	6(1)	4(1)	1(1)
C(26)	22(1)	18(1)	23(1)	5(1)	-2(1)	0(1)
C(27)	27(1)	31(1)	26(1)	7(1)	2(1)	2(1)
C(28)	25(1)	27(1)	31(1)	7(1)	10(1)	8(1)
C(29)	37(1)	23(1)	37(2)	3(1)	8(1)	6(1)
C(30)	30(1)	23(1)	23(1)	8(1)	4(1)	7(1)
C(31)	23(1)	32(1)	29(1)	6(1)	-1(1)	6(1)
C(32)	28(1)	32(1)	44(2)	-3(1)	-1(1)	-5(1)
C(33)	32(1)	52(2)	50(2)	12(2)	-9(1)	10(1)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **3**.

	x	y	z	U(eq)
H(6A)	2539	-121	-5137	44
H(6B)	2367	722	-4337	44
H(6C)	1007	416	-5259	44
H(7A)	-2416	-559	-4373	44
H(7B)	-1483	-1019	-5324	44
H(7C)	-1337	7	-5107	44
H(8A)	-1520	-2403	-2937	50
H(8B)	-2466	-1531	-2829	50
H(8C)	-1487	-1913	-1694	50
H(9A)	1865	-2389	-1305	53
H(9B)	875	-1772	-563	53
H(9C)	2582	-1532	-686	53
H(10A)	4074	27	-2733	48
H(10B)	4321	-984	-2984	48
H(10C)	4093	-661	-1677	48
H(11A)	7533	-3	2127	64
H(11B)	6353	-63	3086	64
H(11C)	7052	857	2783	64
H(12A)	4910	-865	1477	46
H(12B)	5945	-605	468	46
H(12C)	4202	-374	313	46
H(14)	3890(20)	949(16)	2760(20)	16(6)
H(15A)	4620(30)	2301(19)	1470(20)	27(7)
H(15B)	5870(30)	1993(18)	2370(30)	38(8)
H(16)	6730(30)	1312(15)	530(20)	19(6)
H(17A)	4680(30)	1874(16)	-830(20)	19(6)
H(17B)	5020(30)	918(17)	-1040(20)	27(7)
H(18B)	2820(30)	472(15)	-630(20)	19(6)
H(19)	2280(30)	1589(17)	1250(20)	24(7)
H(20A)	1296	404	2119	51
H(20B)	2009	-231	1214	51
H(20C)	676	410	750	51
H(22)	2610(30)	2798(17)	-370(20)	30(7)
H(23)	440(30)	3320(20)	-1860(30)	50(9)
H(24A)	-499	2483	-5672	49
H(24B)	-1119	1582	-5216	49
H(24C)	485	1932	-4686	49
H(25)	-670(30)	3053(17)	-3790(20)	26(7)
H(26)	-1330(30)	1448(16)	-3170(20)	14(6)
H(27A)	-2270(30)	2590(20)	-1560(30)	39(8)
H(27B)	-2870(30)	1650(20)	-1970(30)	40(8)
H(28)	-4770(30)	2664(16)	-2570(20)	17(6)
H(29A)	-2690(30)	3798(17)	-3060(20)	26(7)
H(29B)	-4170(40)	3910(20)	-3780(30)	52(9)
H(30)	-2820(30)	3145(16)	-5230(20)	23(6)
H(32A)	-3872	1205	-5241	52
H(32B)	-5002	1047	-4263	52
H(32C)	-3239	1073	-3888	52

H(33A)	-6451	2357	-4553	68
H(33B)	-5624	2440	-5728	68
H(33C)	-5649	3248	-4845	68