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New fluorinated catalysts for olefin metathesis

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Contents

Experimental Section

General remarks: All solvents were freshly distilled from appropriate drying agents before use. All other reagents were recrystallized or distilled as necessary. Syntheses of ruthenium complexes were performed under an argon atmosphere using a standard Schlenk technique. Analytical TLC was performed with Merck silica gel 60 F254 plates. Visualization was accomplished by UV light (254 and 366 nm), spraying by $Ce(SO_4)_2$ solution in 5% H_2SO_4 or $KMnO_4$ solution in water. Column chromatography was carried out using Merck silica gel 60 (230−400 mesh ASTM) and ethyl acetate/petroleum ether or ethyl acetate/CH_2Cl_2 as eluent. NMR spectra were recorded at room temperature on Bruker AV-300, AV-400, AV-600 spectrometers operating at 300, 400, and 600 MHz for ^{1}H; 101 and 151 MHz for ^{13}C; 282 and 376 MHz for ^{19}F (CF_3CO_2H as reference), and 121 MHz for ^{31}P (85% H_3PO_4 as reference). The chemical shifts are frequency referenced relative to the residual undeuterated solvent peaks.

Synthesis of *N*^{1},*N*^{2}-bis(2,6-dimethylphenyl)ethane-1,2-diamine (1). Compound **1** was synthesized by method that was described in literature.[1] Glyoxal (1.2 g of a 40% aqueous solution, 8.3 mmol, 1 equiv.) was diluted with deionized water (3 mL). Then this solution was poured into a solution of 2,6-dimethylaniline (2 g, 16.5 mmol, 2 equiv.) in isopropyl alcohol (8 mL). The resulting solution was stirred for 24 h at room temperature. A bright yellow precipitate appeared within a few minutes and progressively built up. After 24 h, the suspension was filtered, the precipitate was washed with deionized water (2×5 mL) and dried on the air to yield 1.86 g (85%) of *N*,*N*'-(ethane-1,2-diylidene)bis(2,6-dimethylaniline) as a bright yellow solid. This compound (1.86 g, 7.0 mmol, 1 equiv.) was mixed with THF (20 mL), the resulting yellow suspension was cooled to +5 °C using ice-water bath. Sodium borohydride (1.6 g, 42.0 mmol, 6

[1] M. Hans and L. Delaude, *Org. Synth.*, 2010, **87**, 77.

equiv.) was then added. Then concentrated hydrochloric acid (1.9 mL, 21.0 mmol, 3 equiv.) was added dropwise. White precipitate was appeared. After that, the reaction mixture was stirred for 30 min at 0°C and then transferred into a bigger flask. 3 M aqueous solution of hydrochloric acid (40 mL) was added dropwise. After another 30 min the cooling bath was removed and the reaction mixture was stirred for 1 h at room temperature. Then the precipitate was filtered off and washed with water (3 × 20 mL). The resulting powder was mixed with saturated solution of $NaHCO_3$ (30 mL) and extracted with EtOAc (3 × 10 mL). The combined organic layers were washed with brine, volatiles were removed under reduced pressure to yield 1.3 g diamine **1** (69%) as a while powder.

Synthesis of 2,2'-{4,4'-[ethane-1,2-diylbis(azanediyl)]bis(3,5-dimethyl-4,1-phenylene)}bis-(1,1,1,3,3,3-hexafluoropropan-2-ol) (2). A mixture of diamine **1** (1.3 g, 4.8 mmol, 1 equiv.), hexafluoroacetone sesquihydrate (3.7 g, 19.2 mmol, 4 equiv.), and *p*-TSA (5 mg, 0.03 mmol) was heated at 100 °C for 20 h. After cooling to r.t., water (50 mL) was added and the resulting mixture was extracted with EtOAc (3 × 30 mL). The combined organic layers were washed with water and brine and then dried over $MgSO_4$. The solvent was removed under reduced pressure, and the resulting solid was recrystallized from light petroleum and dried to give 2.5 g (84%) of **2** as white powder. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.29 (s, 4H, Ar*H*), 3.49 (s, 2H, N*H*), 3.27 (s, 4H, (CH_2)$_2$), 2.29 (s, 12H, CH_3); ^{19}F{^{1}H} NMR (282 MHz, $CDCl_3$): δ 2.08 (s). Elemental analysis calcd (%) for $C_{24}H_{24}F_{12}N_2O_2$ (600.44): C 48.01, H 4.03, N 4.67; found: C 47.99, H 4.16, N 4.93.

Synthesis of *N*,*N*'-(ethane-1,2-diyl)bis(2,2,2-trifluoro-*N*-(4-(1,1,1,3,3,3-hexafluoro-2-hydroxypropan-2-yl)-2,6-dimethylphenyl)acetamide) (3). TFAA (0.86 g, 8.2 mmol, 2 equiv.) and pyridine (0.32 g, 8.2 mmol, 2 equiv.) were added sequentially to the solution of diamine **2** (2.45 g, 4.1 mmol, 1 equiv.) in diethyl ether (40 mL) at 0 °C. The reaction mixture was stirred at r.t. for 1 h, and then 5% aqueous solution of hydrochloric acid (20 mL) was added to the mixture. The organic layer was separated; the aqueous layer was extracted with diethyl ether (2 × 20 mL). Combined organic layers were washed with water, dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was recrystallized from petroleum ether to yield 2.76 g (85%) of the corresponding bis-amide as a white solid. ^{1}H NMR (300 MHz, Acetone-d_6): δ 7.63 (d, J = 6.3 Hz, 4H, Ar*H*), 4.14 (s, 4H, (CH_2)$_2$), 2.41 (s, 12H, CH_3); ^{19}F{^{1}H} NMR (282 MHz, Acetone-d_6): δ 6.85 (s), 2.89 (s). Elemental analysis calcd (%) for $C_{28}H_{22}F_{18}N_2O_4$ (792.46): C 42.44, H 2.80, N 3.54; found: C 42.54, H 3.13, N 3.65.

Synthesis of N^1,N^2-bis[4-(1,1,1,3,3,3-hexafluoro-2-methoxypropan-2-yl)-2,6-dimethylphenyl]ethane-1,2-diamine (4). Bis-amide **3** (2.76 g, 3.5 mmol, 1 equiv.) was dissolved in dry DMF (40 mL). MeI (1.3 g, 9.1 mmol, 2.6 equiv.) and anhydrous K_2CO_3 (1.93 g, 14 mmol, 4 equiv.) were added, and the resulting mixture was heated for 1.5 h at 80 °C. Then, after cooling to r.t., 20 mL of brine was added. The resulting mixture was extracted with EtOAc (3 × 15 mL). Combined organic layers were dried over $MgSO_4$, filtered, and concentrated under reduced pressure to afford 2.17 g (76%) of corresponding methylated product *N*,*N*'-(ethane-1,2-diyl)bis{2,2,2-trifluoro-*N*-[4-(1,1,1,3,3,3-hexafluoro-2-methoxypropan-2-yl)-2,6-dimethylphenyl]acetamide} as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.36 (s, 4H, Ar*H*), 4.03 (s, 4H, (C*H*$_2$)$_2$), 3.51 (s, 6H, OC*H*$_3$), 2.33 (s, 12H, C*H*$_3$); ^{19}F{^{1}H} NMR (282 MHz, $CDCl_3$): δ 7.05 (s), 6.73 (s); ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.2 (q, $^2J_{C,F}$ = 37 Hz), 139.4, 137.2, 129.4, 128.9, 122.3 (q, $^1J_{C,F}$ = 291 Hz), 115.8 (q, $^1J_{C,F}$ = 288 Hz), 83.5-81.9 (m), 54. 7, 49.3, 18.8. Elemental analysis calcd (%) for $C_{30}H_{26}F_{18}N_2O_4$ (820.51): C 43.91, H 3.19, N 3.41; found: C 43.58, H 3.20, N 3.46. Then a mixture of this product (2.17 g, 2.6 mmol, 1 equiv.), 18-crown-6 (5 mg, 0.02 mmol), and a solution of KOH (14.6 g, 260 mmol, 100 equiv.) in water (20 mL) was stirred vigorously and heated in DMSO (40 mL) at 130 °C for 1.5 h. After that water (50 mL) was added, and the crude product was extracted with EtOAc (3 × 30 mL). Combined organic layers were washed with 20 mL of water, dried over $MgSO_4$, and concentrated. The product was purified by column chromatography using EtOAc/light petroleum (1:5) as eluent to yield 1.32 g (80%) of diamine **4** as a white powder. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.16 (s, 4H, Ar*H*), 3.53 (bs, 2H, N*H*), 3.47 (s, 6H, OC*H*$_3$), 3.30 (s, 4H, (C*H*$_2$)$_2$), 2.30 (s, 12H, C*H*$_3$); ^{19}F{^{1}H} NMR (282 MHz, $CDCl_3$): δ 6.73 (s); ^{13}C NMR (126 MHz, $CDCl_3$): δ 147.6, 128.9, 128.8, 122.7 (q, $^2J_{C,F}$ = 289 Hz), 120.1, 83.0 (quint, $^1J_{C,F}$ = 28 Hz), 54.2, 48.3, 19.2. Elemental analysis calcd (%) for $C_{26}H_{28}F_{12}N_2O_2$ (628.49): C 49.69, H 4.49, N 4.46; found: C 49.84, H 4.74, N 4.37.

Synthesis of 1,3-bis[4-(1,1,1,3,3,3-hexafluoro-2-methoxypropan-2-yl)-2,6-dimethylphenyl]-4,5-dihydroimidazolium chloride (5). Concentrated HCl (5 mL, 60 mmol) was added to the solution of diamine **4** (1.32 g, 2.1 mmol) in MeOH (60 mL) and stirred for 10 min. The solution was evaporated under reduced pressure. This operation was repeated two more times. To the resulting solid, $CH(OEt)_3$ (15 g, 100 mmol, 50 equiv.) was added, and the mixture was heated at 100 °C for 4 h. Then, the excess of $CH(OEt)_3$ was removed under vacuum and the resulting solid was washed with 20 mL of Et_2O. The recrystallization from EtOAc gave pure imidazolinium chloride **5** (1 g, 71%) as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.97 (s, 1H, C*H*), 7.30 (s, 4H, Ar*H*), 4.54 (s, 4H, (C*H*$_2$)$_2$), 3.44 (s, 6H, OC*H*$_3$), 2.43 (s, 12H, C*H*$_3$); ^{19}F{^{1}H} NMR (282 MHz, $CDCl_3$): δ 6.30 (s); ^{13}C NMR (101 MHz, $CDCl_3$): δ 160.4, 136.4, 134.6, 130.4, 129.1,

122.2 (q, $^{1}J_{C,F}$ = 289 Hz), 82.5 (quint, $^{2}J_{C,F}$ = 28 Hz), 54.7, 51.8, 18.5. Elemental analysis calcd (%) for $C_{27}H_{27}ClF_{12}N_2O_2$ (674.95): C 48.05, H 4.03, N 4.15; found: C 47.74, H 4.10, N 4.07.

Synthesis of benzylidene{1,3-bis[4-(1,1,1,3,3,3-hexafluoro-2-methoxypropan-2-yl)-2,6-dimethylphenyl]-4,5-dihydroimidazol-2-ylidene}(tricyclohexylphosphine)ruthenium(II) dichloride (6a). In a flame-dried Schlenk flask compound **5** (300 mg, 0.44 mmol) was mixed with 20 mL of anhydrous toluene. The mixture was cooled to 0°C, degassed three times, and then KHMDS (460 μL of 1 M solution in THF, 0.46 mmol) was added to the mixture under an argon atmosphere. The reaction mixture was stirred for 30 min; then **G-I** (305 mg, 0.37 mmol) was added and the mixture was stirred for 2 h at room temperature. After removal of volatiles, the residue was purified by column chromatography on silica gel in a gradient manner using EtOAc/petroleum ether (1:8−1:3) as eluent under an argon atmosphere to yield 130 mg (30%) of complex **6a** as a brown solid. ^{1}H NMR (600 MHz, C_6D_6): δ 19.55 (s, 1H, CHPh), 8.33 (bs, 2H, ArH), 7.59 (s, 2H, ArH), 7.15–6.92 (m, 5H, ArH), 3.30 (s, 3H, OCH_3), 3.10 (t, $^{3}J_{H,H}$ = 10.2 Hz, 2H, CH_2), 3.01 (s, 3H, OCH_3), 2.93 (t, $^{3}J_{H,H}$ = 10.2 Hz, 2H, CH_2), 2.76 (s, 6H, CH_3), 2.43 (s, 6H, CH_3), 2.04 (q, $J_{H,P}$ = 11.7 Hz, 3H, PCy_3), 1.68–1.50 (m, 16H, PCy_3), 1.37–1.26 (m, 6H, PCy_3), 1.11–1.00 (m, 8H, PCy_3); ^{19}F{^{1}H} NMR (376 MHz, C_6D_6): δ 7.49 (s); ^{31}P NMR (162 MHz, C_6D_6): δ 20.93 (s); ^{13}C NMR (151 MHz, C_6D_6): δ 299.7 (br. s), 220.2 (d, $^{2}J_{C,P}$ = 79.3 Hz), 152.8, 152.7, 142.2, 141.0, 139.9, 138.8, 123.3 (d, $^{1}J_{C,F}$ = 290 Hz), 123.1 (d, $^{1}J_{C,F}$ = 289 Hz), 83.4 (m), 54.5, 54.3, 51.3, 35.9, 35.5, 33.0 (d, $^{1}J_{C,P}$ = 16 Hz), 29.1, 27.9 (d, $^{3}J_{C,P}$=10 Hz), 27.2 (d, $^{2}J_{C,P}$=12 Hz), 20.8, 19.4. Elemental analysis calcd (%) for $C_{52}H_{65}Cl_2F_{12}N_2O_2PRu$ (1181.02): C 52.88, H 5.55, N 2.37; found: C 53.04, H 5.56, N 2.44.

Synthesis of (2-isopropylbenzylidene){1,3-bis[4-(1,1,1,3,3,3-hexafluoro-2-methoxypropan-2-yl)-2,6-dimethylphenyl]-4,5-dihydroimidazol-2-ylidene}ruthenium(II) dichloride (6b). In a flame-dried Schlenk flask compound **5** (360 mg, 0.54 mmol) was mixed with 20 mL of anhydrous toluene. The mixture was cooled to 0°C and degassed three times; then KHMDS (560 μL of 1 M solution in THF, 0.56 mmol) was added to the mixture under an argon atmosphere. The reaction mixture was stirred for 30 min at r.t.; then **H-I** (270 g, 0.45 mmol) was added and mixture was stirred for 1 h at 60°C. After removal of volatiles, the residue was purified by column chromatography on silica gel using EtOAc/petroleum ether (1:3) as eluent to yield 140 mg (32%) of complex **6b** as a green solid. Suitable for X-ray crystals were grown by slow diffusion of hexane vapors in CH_2Cl_2 solution. ^{1}H NMR (600 MHz, C_6D_6): δ 16.53 (s, 1H, CHAr), 7.61 (s, 4H, ArH), 7.12 (d, $J_{H,H}$ = 7.6 Hz, 1H, ArH), 7.07 (t, $J_{H,H}$ = 7.8 Hz, 1H, ArH), 6.65 (t, $J_{H,H}$ = 7.5 Hz, 1H, ArH), 6.29 (d, $J_{H,H}$ = 8.2 Hz, 1H, ArH), 4.45 (hept, $^{3}J_{H,H}$ = 6.1 Hz, 1H,

O^{i}Pr CH), 3.26 (s, 6H, OCH_3), 3.22 (s, 4H, $(CH_2)_2$), 2.49 (s, 12H, CH_3), 1.27 (d, $^{3}J_{H,H}$ = 6.2 Hz, 6H, O^{i}Pr CH_3); $^{19}F\{^{1}H\}$ NMR (282 MHz, C_6D_6): δ 7.52 (s); ^{13}C NMR (151 MHz, C_6D_6): δ 301. 3, 213.2, 152.8, 145.6, 140.9, 129.7, 128.9, 128.8, 128.4, 123.3 (q, $^{2}J_{C,F}$ = 290 Hz), 122.4, 122.3, 113.3, 83.5 (quint, $^{1}J_{C,F}$ = 29 Hz), 75.3, 54.3, 51.0, 21.4. Elemental analysis calcd (%) for $C_{37}H_{38}Cl_2F_{12}N_2O_3Ru$ (958.67): C 46.36, H 4.00, N 2.92; found: C 46.65, H 4.21, N 2.94.

Crystallographic data for 6b.

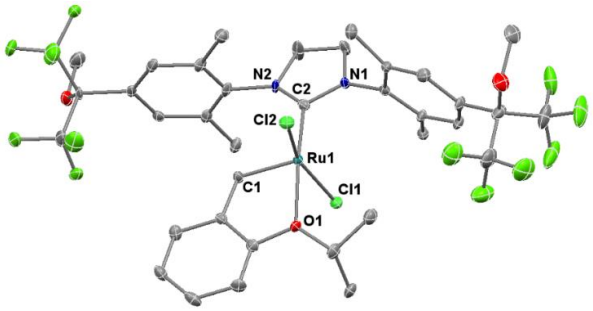

Figure S1 Molecular structure of complex **6b.** Thermal ellipsoids are drawn at 30% probability. Hydrogen atoms are omitted for clarity.

Table S1 Selected bond lengths and angles for **6b.**

Bond Lengths (Å)			
Ru(1)–C(1)	1.823(5)	Ru(1)–Cl(1)	2.332(2)
Ru(1)–C(2)	1.978(5)	Ru(1)–Cl(2)	2.335(1)
Ru(1)–O(1)	2.253(4)	C(2)–N(1)	1.357(7)
		C(2)–N(2)	1.344(7)
Bond Angles (°)			
C(1)–Ru(1)–O(1)	79.4(2)	O(1)–Ru(1)–Cl(1)	86.0(1)
C(1)–Ru(1)–C(2)	102.6(2)	O(1)–Ru(1)–Cl(2)	86.6(1)
C(2)–Ru(1)–O(1)	174.8(2)	C(2)–Ru(1)–Cl(1)	88.9(2)
C(1)–Ru(1)–Cl(1)	102.2(2)	C(2)–Ru(1)–Cl(2)	97.8(2)
C(1)–Ru(1)–Cl(2)	96.6(2)	Cl(1)–Ru(1)–Cl(2)	158.20(6)
		N(1)–C(2)–N(2)	106.7(4)

$C_{37}H_{38}Cl_2F_{12}N_2O_3Ru$; M = 958.67. APEXII, Bruker-AXS diffractometer, Mo-Kα radiation (λ = 0.71073 E), T = 150(2) K; orthorhombic $Pc2_1b$ (I.T.#29), a = 11.7016(12), b = 13.0525(14), c = 26.190(3) E, V = 4000.1(7) E^3.Z = 4, d = 1.588 g.cm-3, μ = 0.620 mm-1. The structure was solved by direct methods using the *SIR97* program [1], and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*) [2] with the aid of the *WINGX* [3] program. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 7338 unique intensities and 516 parameters converged at $\omega R(F^2)$ = 0.1105 ($R(F)$ = 0.0516) for 5541 observed reflections with $I > 2\sigma(I)$.

[1] A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori and R. Spagna, *J. Appl. Crystallogr*., 1999, **32**, 115.
[2] G.M. Sheldrick, *Acta Crystallogr*., 2008, **A64**, 112.
[3] L. J. Farrugia, *J. Appl. Crystallogr*., 2012, **45**, 849.

Structural data

Empirical formula	C37 H38 Cl2 F12 N2 O3 Ru
Formula weight	956.65
Temperature	150(2) K
Wavelength	0.71073 E
Crystal system, space group	orthorhombic, P c 21 b
Unit cell dimensions	a = 11.7016(12) E, α = 90 °
	b = 13.0525(14) E, β = 90 °
	c = 26.190(3) E, γ = 90 °
Volume	4000.1(7) E3
Z, Calculated density	4, 1.588 (g.cm-3)
Absorption coefficient	0.620 mm-1
F(000)	1928
Crystal size	0.35 x 0.32 x 0.12 mm
Crystal color	yellow
Theta range for data collection	2.91 to 27.48 °
h_min, h_max	-10, 15
k_min, k_max	-10, 16
l_min, l_max	-28, 33
Reflections collected / unique	19163 / 7338 [R(int)a = 0.0646]
Reflections [I>2σ]	5541
Completeness to theta_max	0.995
Absorption correction type	multi-scan
Max. and min. transmission	0.928 , 0.766
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	7338 / 1 / 516
bGoodness-of-fit	1.031
Final R indices [I>2σ]	R1c = 0.0516, wR2d = 0.1105
R indices (all data)	R1c = 0.075, wR2d = 0.1209
Largest diff. peak and hole	0.57 and -0.405 e-.E-3

aRint = ∑ |Fo2 - < Fo2>| / ∑[Fo2]

bS = {∑ [w(Fo2 - Fc2)2] / (n - p)}1/2

cR1 = ∑ | |Fo| - |Fc| | / ∑ |Fo|

dwR2 = {∑ [w(Fo2 - Fc2)2] / ∑ [w(Fo2)2]}1/2

w = 1 / [σ(Fo2) + aP2 + bP] where P = [2Fc2 + MAX(Fo2, 0)] /3

Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters (E2 x 103). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	occ.	U(eq)
C1	0.2938(5)	0.3301(4)	0.4505(2)	1	0.0227(13)
H1	0.3306	0.3511	0.4199	1	0.027
C2	0.2617(5)	0.2231(5)	0.4580(2)	1	0.0219(14)
C3	0.2767(5)	0.1481(5)	0.4204(3)	1	0.0286(15)
H3	0.3086	0.1665	0.3884	1	0.034
C4	0.2453(5)	0.0467(5)	0.4295(3)	1	0.0340(16)
H4	0.2543	-0.004	0.4038	1	0.041
C5	0.2004(5)	0.0216(5)	0.4770(3)	1	0.0355(16)
H5	0.1813	-0.0478	0.4838	1	0.043
C6	0.1827(5)	0.0947(5)	0.5148(3)	1	0.0313(15)
H6	0.1496	0.0763	0.5466	1	0.038
C7	0.2143(5)	0.1952(5)	0.5049(2)	1	0.0251(14)
O8	0.1993(3)	0.2774(3)	0.53754(16)	1	0.0255(9)
C9	0.1553(5)	0.2615(5)	0.5897(2)	1	0.0318(15)
H9	0.0898	0.2124	0.5884	1	0.038
C10	0.2488(6)	0.2169(6)	0.6234(3)	1	0.0365(17)
H10A	0.2762	0.1525	0.6086	1	0.055
H10B	0.2181	0.2038	0.6576	1	0.055
H10C	0.3122	0.2656	0.6258	1	0.055
C11	0.1134(6)	0.3624(5)	0.6084(3)	1	0.0393(18)
H11A	0.1781	0.4094	0.6124	1	0.059
H11B	0.0753	0.3533	0.6415	1	0.059
H11C	0.059	0.3909	0.5838	1	0.059
C15	0.3287(4)	0.5507(4)	0.4731(2)	1	0.0185(12)
N16	0.3287(4)	0.6381(3)	0.50117(18)	1	0.0183(10)
C17	0.3971(6)	0.7207(5)	0.4787(3)	1	0.0327(16)
H17	0.4064	0.7888	0.4908	1	0.039
C18	0.4484(6)	0.6733(5)	0.4326(3)	1	0.045(2)
H18	0.5015	0.702	0.4092	1	0.055
N19	0.3954(4)	0.5684(3)	0.43226(18)	1	0.0216(11)
C21	0.4040(5)	0.5104(5)	0.3862(2)	1	0.0234(13)
C22	0.3167(5)	0.5162(5)	0.3508(2)	1	0.0246(13)
C23	0.3284(5)	0.4648(4)	0.3040(2)	1	0.0278(14)
H23	0.2688	0.468	0.2794	1	0.033
C24	0.4277(5)	0.4088(4)	0.2935(2)	1	0.0245(13)
C25	0.5147(5)	0.4030(4)	0.3296(2)	1	0.0236(13)
H25	0.5822	0.3653	0.3222	1	0.028
C26	0.5031(5)	0.4526(4)	0.3768(2)	1	0.0243(13)
C27	0.2122(5)	0.5789(5)	0.3606(3)	1	0.0362(16)
H27A	0.1713	0.5512	0.3902	1	0.054
H27B	0.1623	0.5768	0.3305	1	0.054
H27C	0.2344	0.65	0.3675	1	0.054

C28	0.5947(5)	0.4422(5)	0.4171(2)	1	0.0298(14)
H28A	0.6251	0.5101	0.4255	1	0.045
H28B	0.6565	0.3987	0.4042	1	0.045
H28C	0.5618	0.4111	0.4479	1	0.045
C29	0.4471(6)	0.3514(4)	0.2428(2)	1	0.0285(14)
O30	0.5626(4)	0.3478(3)	0.22855(17)	1	0.0388(12)
C31	0.6158(7)	0.4437(6)	0.2157(3)	1	0.052(2)
H31A	0.5924	0.4643	0.1812	1	0.078
H31B	0.699	0.436	0.2168	1	0.078
H31C	0.5921	0.4963	0.2402	1	0.078
C32	0.3763(7)	0.3951(5)	0.1989(3)	1	0.0417(18)
F33	0.4122(4)	0.3620(3)	0.15339(15)	1	0.0598(13)
F34	0.3792(3)	0.4977(3)	0.19651(14)	1	0.0386(10)
F35	0.2639(4)	0.3686(4)	0.20297(18)	1	0.0621(14)
C36	0.4216(8)	0.2377(5)	0.2511(3)	1	0.050(2)
F38	0.4278(5)	0.1862(3)	0.20632(16)	1	0.0710(16)
F39	0.4925(4)	0.1946(3)	0.28227(15)	1	0.0504(11)
F40	0.3137(4)	0.2262(3)	0.27068(19)	1	0.0680(14)
C41	0.2630(5)	0.6555(4)	0.5465(2)	1	0.0213(14)
C42	0.3152(5)	0.6532(4)	0.5943(2)	1	0.0226(13)
C43	0.2455(5)	0.6676(5)	0.6370(3)	1	0.0301(15)
H43	0.279	0.6639	0.67	1	0.036
C44	0.1297(5)	0.6871(5)	0.6331(2)	1	0.0277(14)
C45	0.0820(5)	0.6961(5)	0.5840(3)	1	0.0302(14)
H45	0.0027	0.7106	0.5809	1	0.036
C46	0.1459(5)	0.6845(4)	0.5407(2)	1	0.0214(12)
C47	0.4418(5)	0.6420(4)	0.5996(2)	1	0.0257(14)
H47A	0.4724	0.607	0.5695	1	0.038
H47C	0.4768	0.7099	0.6026	1	0.038
C48	0.0957(5)	0.7075(5)	0.4896(2)	1	0.0310(15)
H48A	0.0902	0.6441	0.4696	1	0.047
H48B	0.1446	0.7566	0.4715	1	0.047
H48C	0.0192	0.7369	0.4939	1	0.047
C49	0.0516(6)	0.6983(6)	0.6791(3)	1	0.0392(17)
O50	-0.0564(5)	0.7417(4)	0.6691(2)	1	0.0584(13)
C51	-0.0506(7)	0.8509(6)	0.6541(3)	1	0.0584(13)
H51A	0.0273	0.8674	0.643	1	0.088
H51B	-0.0711	0.894	0.6833	1	0.088
H51C	-0.1039	0.8636	0.626	1	0.088
C52	0.0089(8)	0.5883(7)	0.6962(3)	1	0.060(2)
F53	-0.0542(4)	0.5471(4)	0.6612(2)	1	0.0722(15)
F54	0.0985(4)	0.5263(4)	0.70557(19)	1	0.0753(16)
F55	-0.0535(5)	0.5928(5)	0.7391(2)	1	0.0828(17)
C56	0.1102(7)	0.7493(8)	0.7234(3)	1	0.060(2)
F57	0.1854(4)	0.6938(5)	0.7475(2)	1	0.0879(18)

F58	0.0344(5)	0.7850(5)	0.7588(2)	1	0.092(2)
F59	0.1652(4)	0.8369(5)	0.7070(2)	1	0.0782(16)
Cl1	0.42125(12)	0.40684(11)	0.55387(6)	1	0.0279(3)
Cl2	0.07267(12)	0.45271(11)	0.47737(6)	1	0.0286(3)
Ru1	0.26241(3)	0.42274(7)	0.500656(18)	1	0.01869(11)

Anisotropic displacement parameters (E2)

The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [h2 a*2 U11 + ... + 2 h k a* b* U12].

Atom	U11	U22	U33	U23	U13	U12
C1	0.033(3)	0.017(3)	0.018(3)	-0.001(2)	0.007(3)	-0.002(2)
C2	0.023(3)	0.019(3)	0.024(4)	-0.001(3)	-0.001(3)	0.002(2)
C3	0.025(3)	0.031(4)	0.029(4)	-0.005(3)	0.006(3)	-0.007(3)
C4	0.040(4)	0.023(3)	0.039(4)	-0.009(3)	0.007(3)	0.000(3)
C5	0.034(3)	0.019(3)	0.054(5)	-0.003(3)	0.004(3)	-0.002(3)
C6	0.037(4)	0.023(3)	0.034(4)	0.008(3)	0.005(3)	-0.010(3)
C7	0.024(3)	0.023(3)	0.028(4)	-0.001(3)	0.000(3)	-0.002(2)
O8	0.038(2)	0.023(2)	0.016(2)	0.0024(18)	0.0048(19)	0.0012(19)
C9	0.033(3)	0.043(4)	0.020(3)	0.003(3)	0.009(3)	-0.001(3)
C10	0.055(5)	0.040(4)	0.015(4)	0.003(3)	0.002(3)	0.003(3)
C11	0.048(4)	0.046(4)	0.024(4)	0.001(3)	0.008(3)	0.008(3)
C15	0.027(3)	0.017(3)	0.011(3)	-0.001(2)	-0.005(3)	-0.002(2)
N16	0.027(2)	0.014(2)	0.015(3)	-0.002(2)	0.006(2)	-0.0028(18)
C17	0.054(4)	0.017(3)	0.027(4)	-0.006(3)	0.019(3)	-0.009(3)
C18	0.076(5)	0.031(4)	0.030(4)	-0.010(3)	0.021(4)	-0.038(4)
N19	0.033(3)	0.020(2)	0.011(3)	-0.005(2)	0.006(2)	-0.009(2)
C21	0.029(3)	0.030(3)	0.011(3)	0.001(3)	0.007(2)	-0.012(3)
C22	0.025(3)	0.032(3)	0.017(3)	0.003(3)	0.006(3)	-0.006(3)
C23	0.039(4)	0.028(3)	0.017(3)	0.001(3)	-0.003(3)	-0.011(3)
C24	0.044(3)	0.015(3)	0.014(3)	0.001(3)	0.006(2)	-0.009(3)
C25	0.035(3)	0.014(3)	0.022(3)	0.001(2)	0.003(2)	-0.003(2)
C26	0.033(3)	0.023(3)	0.017(3)	0.001(2)	0.001(2)	-0.012(2)
C27	0.044(4)	0.036(4)	0.028(4)	0.003(3)	0.004(3)	0.007(3)
C28	0.037(3)	0.035(4)	0.018(3)	-0.001(3)	0.000(2)	-0.005(3)
C29	0.054(4)	0.016(3)	0.015(3)	-0.009(3)	0.002(3)	-0.008(3)
O30	0.062(3)	0.031(2)	0.023(3)	-0.002(2)	0.018(2)	0.002(2)
C31	0.083(6)	0.044(5)	0.028(4)	0.007(4)	0.007(4)	-0.017(4)
C32	0.065(5)	0.034(4)	0.026(4)	-0.005(3)	0.001(3)	-0.004(3)
F33	0.118(4)	0.048(3)	0.014(2)	-0.0033(19)	-0.001(2)	0.017(2)
F34	0.068(3)	0.027(2)	0.021(2)	0.0024(16)	0.0006(19)	0.0015(18)
F35	0.080(3)	0.066(3)	0.040(3)	-0.007(2)	-0.012(2)	-0.022(2)
C36	0.096(7)	0.029(4)	0.024(4)	-0.006(3)	-0.005(4)	-0.012(4)

F38	0.158(5)	0.022(2)	0.033(3)	-0.0075(19)	-0.026(3)	-0.006(3)
F39	0.100(3)	0.023(2)	0.029(2)	0.0042(18)	-0.018(2)	-0.009(2)
F40	0.095(4)	0.049(3)	0.059(3)	0.002(2)	0.006(3)	-0.036(3)
C41	0.029(3)	0.015(3)	0.020(3)	-0.001(3)	0.002(3)	-0.003(2)
C42	0.028(3)	0.028(3)	0.012(3)	-0.001(3)	0.000(3)	0.004(3)
C43	0.042(4)	0.035(4)	0.013(3)	0.000(3)	-0.005(3)	0.008(3)
C44	0.034(3)	0.038(4)	0.012(3)	-0.002(3)	0.007(3)	0.008(3)
C45	0.028(3)	0.033(3)	0.030(4)	0.002(3)	0.004(3)	0.001(3)
C46	0.028(3)	0.020(3)	0.016(3)	0.000(2)	-0.001(3)	0.005(2)
C47	0.029(3)	0.026(3)	0.022(3)	-0.004(3)	-0.001(3)	0.004(3)
C48	0.031(3)	0.036(4)	0.026(4)	-0.005(3)	0.003(3)	-0.001(3)
C49	0.047(4)	0.050(4)	0.020(4)	0.006(3)	0.002(3)	0.022(3)
O50	0.073(3)	0.056(3)	0.046(3)	-0.007(2)	0.021(2)	0.031(3)
C51	0.073(3)	0.056(3)	0.046(3)	-0.007(2)	0.021(2)	0.031(3)
C52	0.080(7)	0.075(6)	0.025(5)	0.005(4)	0.020(5)	0.015(5)
F53	0.077(3)	0.085(4)	0.055(3)	0.006(3)	0.007(3)	-0.020(3)
F54	0.088(4)	0.081(4)	0.057(3)	0.023(3)	0.022(3)	0.041(3)
F55	0.101(4)	0.095(4)	0.052(4)	0.017(3)	0.037(3)	0.005(3)
C56	0.061(6)	0.095(7)	0.024(5)	-0.015(5)	0.007(4)	-0.003(5)
F57	0.085(3)	0.151(5)	0.028(3)	-0.017(3)	-0.004(3)	0.048(4)
F58	0.080(3)	0.147(6)	0.048(4)	-0.047(4)	0.010(3)	0.023(4)
F59	0.086(4)	0.090(4)	0.059(4)	-0.048(3)	0.005(3)	-0.006(3)
Cl1	0.0326(7)	0.0258(8)	0.0253(8)	-0.0009(7)	-0.0063(6)	0.0033(7)
Cl2	0.0242(7)	0.0283(8)	0.0333(9)	0.0046(7)	0.0009(6)	-0.0004(6)
Ru1	0.02349(19)	0.01687(18)	0.01570(19)	-0.00073(19)	0.0032(2)	-0.0008(3)

Bond lengths [E]

C1 - C2	= 1.459(8)
C1 - Ru1	= 1.823(6)
C1 - H1	= 0.95
C2 - C7	= 1.394(8)
C2 - C3	= 1.400(8)
C3 - C4	= 1.393(9)
C3 - H3	= 0.95
C4 - C5	= 1.389(10)
C4 - H4	= 0.95
C5 - C6	= 1.391(9)
C5 - H5	= 0.95
C6 - C7	= 1.387(8)
C6 - H6	= 0.95
C7 - O8	= 1.384(7)
O8 - C9	= 1.476(7)
O8 - Ru1	= 2.253(4)

C9 - C11 = 1.488(9)
C9 - C10 = 1.521(9)
C9 - H9 = 1
C10 - H10A = 0.98
C10 - H10B = 0.98
C10 - H10C = 0.98
C11 - H11A = 0.98
C11 - H11B = 0.98
C11 - H11C = 0.98
C15 - N19 = 1.344(7)
C15 - N16 = 1.357(7)
C15 - Ru1 = 1.978(5)
N16 - C41 = 1.433(7)
N16 - C17 = 1.467(7)
C17 - C18 = 1.483(9)
C17 - H17 = 0.95
C18 - N19 = 1.503(7)
C18 - H18 = 0.95
N19 - C21 = 1.429(7)
C21 - C22 = 1.381(8)
C21 - C26 = 1.405(8)
C22 - C23 = 1.404(8)
C22 - C27 = 1.494(8)
C23 - C24 = 1.400(8)
C23 - H23 = 0.95
C24 - C25 = 1.391(8)
C24 - C29 = 1.541(8)
C25 - C26 = 1.402(8)
C25 - H25 = 0.95
C26 - C28 = 1.512(8)
C27 - H27A = 0.98
C27 - H27B = 0.98
C27 - H27C = 0.98
C28 - H28A = 0.98
C28 - H28B = 0.98
C28 - H28C = 0.98
C29 - O30 = 1.403(8)
C29 - C32 = 1.527(9)
C29 - C36 = 1.529(9)
O30 - C31 = 1.438(8)
C31 - H31A = 0.98
C31 - H31B = 0.98
C31 - H31C = 0.98
C32 - F33 = 1.337(8)
C32 - F34 = 1.341(7)

C32 - F35 = 1.364(8)
C36 - F39 = 1.294(9)
C36 - F38 = 1.353(8)
C36 - F40 = 1.372(9)
C41 - C42 = 1.394(8)
C41 - C46 = 1.429(8)
C42 - C43 = 1.397(8)
C42 - C47 = 1.495(8)
C43 - C44 = 1.383(8)
C43 - H43 = 0.95
C44 - C45 = 1.406(8)
C44 - C49 = 1.519(8)
C45 - C46 = 1.367(8)
C45 - H45 = 0.95
C46 - C48 = 1.495(8)
C47 - H47A = 0.98
C47 - H47B = 0.98
C47 - H47C = 0.98
C48 - H48A = 0.98
C48 - H48B = 0.98
C48 - H48C = 0.98
C49 - O50 = 1.410(8)
C49 - C56 = 1.503(11)
C49 - C52 = 1.584(12)
O50 - C51 = 1.480(9)
C51 - H51A = 0.98
C51 - H51B = 0.98
C51 - H51C = 0.98
C52 - F53 = 1.294(10)
C52 - F55 = 1.340(9)
C52 - F54 = 1.347(9)
C56 - F57 = 1.304(10)
C56 - F58 = 1.365(9)
C56 - F59 = 1.380(10)
Cl1 - Ru1 = 2.3325(14)
Cl2 - Ru1 = 2.3354(15)

Angles [°]

C2 - C1 - Ru1 = 119.0(4)
C2 - C1 - H1 = 120.5
Ru1 - C1 - H1 = 120.5
C7 - C2 - C3 = 119.0(6)
C7 - C2 - C1 = 118.2(6)
C3 - C2 - C1 = 122.8(6)

C4 - C3 - C2 = 120.8(6)
C4 - C3 - H3 = 119.6
C2 - C3 - H3 = 119.6
C5 - C4 - C3 = 118.4(6)
C5 - C4 - H4 = 120.8
C3 - C4 - H4 = 120.8
C4 - C5 - C6 = 122.1(6)
C4 - C5 - H5 = 118.9
C6 - C5 - H5 = 118.9
C7 - C6 - C5 = 118.3(6)
C7 - C6 - H6 = 120.8
C5 - C6 - H6 = 120.8
O8 - C7 - C6 = 125.6(6)
O8 - C7 - C2 = 113.1(5)
C6 - C7 - C2 = 121.2(6)
C7 - O8 - C9 = 120.6(4)
C7 - O8 - Ru1 = 110.2(3)
C9 - O8 - Ru1 = 129.1(3)
O8 - C9 - C11 = 107.2(5)
O8 - C9 - C10 = 109.9(5)
C11 - C9 - C10 = 112.7(6)
O8 - C9 - H9 = 109
C11 - C9 - H9 = 109
C10 - C9 - H9 = 109
C9 - C10 - H10A = 109.5
C9 - C10 - H10B = 109.5
H10A - C10 - H10B = 109.5
C9 - C10 - H10C = 109.5
H10A - C10 - H10C = 109.5
H10B - C10 - H10C = 109.5
C9 - C11 - H11A = 109.5
C9 - C11 - H11B = 109.5
H11A - C11 - H11B = 109.5
C9 - C11 - H11C = 109.5
H11A - C11 - H11C = 109.5
H11B - C11 - H11C = 109.5
N19 - C15 - N16 = 106.7(4)
N19 - C15 - Ru1 = 131.5(4)
N16 - C15 - Ru1 = 120.8(4)
C15 - N16 - C41 = 125.6(5)
C15 - N16 - C17 = 113.6(5)
C41 - N16 - C17 = 120.6(5)
N16 - C17 - C18 = 103.9(5)
N16 - C17 - H17 = 128
C18 - C17 - H17 = 128

C17 - C18 - N19 = 102.6(5)
C17 - C18 - H18 = 128.7
N19 - C18 - H18 = 128.7
C15 - N19 - C21 = 128.5(5)
C15 - N19 - C18 = 113.0(5)
C21 - N19 - C18 = 117.3(5)
C22 - C21 - C26 = 121.5(5)
C22 - C21 - N19 = 119.1(5)
C26 - C21 - N19 = 119.3(5)
C21 - C22 - C23 = 119.2(5)
C21 - C22 - C27 = 121.3(6)
C23 - C22 - C27 = 119.5(6)
C24 - C23 - C22 = 120.1(6)
C24 - C23 - H23 = 119.9
C22 - C23 - H23 = 119.9
C25 - C24 - C23 = 120.1(5)
C25 - C24 - C29 = 116.8(5)
C23 - C24 - C29 = 123.1(5)
C24 - C25 - C26 = 120.2(5)
C24 - C25 - H25 = 119.9
C26 - C25 - H25 = 119.9
C25 - C26 - C21 = 118.9(5)
C25 - C26 - C28 = 120.4(5)
C21 - C26 - C28 = 120.7(5)
C22 - C27 - H27A = 109.5
C22 - C27 - H27B = 109.5
H27A - C27 - H27B = 109.5
C22 - C27 - H27C = 109.5
H27A - C27 - H27C = 109.5
H27B - C27 - H27C = 109.5
C26 - C28 - H28A = 109.5
C26 - C28 - H28B = 109.5
H28A - C28 - H28B = 109.5
C26 - C28 - H28C = 109.5
H28A - C28 - H28C = 109.5
H28B - C28 - H28C = 109.5
O30 - C29 - C32 = 109.6(5)
O30 - C29 - C36 = 101.2(6)
C32 - C29 - C36 = 111.3(6)
O30 - C29 - C24 = 112.8(5)
C32 - C29 - C24 = 112.7(5)
C36 - C29 - C24 = 108.8(5)
C29 - O30 - C31 = 116.8(5)
O30 - C31 - H31A = 109.5
O30 - C31 - H31B = 109.5

H31A - C31 - H31B = 109.5
O30 - C31 - H31C = 109.5
H31A - C31 - H31C = 109.5
H31B - C31 - H31C = 109.5
F33 - C32 - F34 = 105.8(6)
F33 - C32 - F35 = 106.9(6)
F34 - C32 - F35 = 106.3(6)
F33 - C32 - C29 = 112.3(6)
F34 - C32 - C29 = 113.3(6)
F35 - C32 - C29 = 111.8(6)
F39 - C36 - F38 = 107.3(6)
F39 - C36 - F40 = 107.8(6)
F38 - C36 - F40 = 108.6(6)
F39 - C36 - C29 = 112.7(6)
F38 - C36 - C29 = 110.4(6)
F40 - C36 - C29 = 109.8(6)
C42 - C41 - C46 = 121.4(6)
C42 - C41 - N16 = 120.4(5)
C46 - C41 - N16 = 117.9(5)
C41 - C42 - C43 = 117.4(5)
C41 - C42 - C47 = 121.3(5)
C43 - C42 - C47 = 121.1(5)
C44 - C43 - C42 = 122.5(6)
C44 - C43 - H43 = 118.8
C42 - C43 - H43 = 118.8
C43 - C44 - C45 = 118.2(5)
C43 - C44 - C49 = 123.2(6)
C45 - C44 - C49 = 118.6(5)
C46 - C45 - C44 = 122.1(6)
C46 - C45 - H45 = 118.9
C44 - C45 - H45 = 118.9
C45 - C46 - C41 = 117.8(5)
C45 - C46 - C48 = 120.4(5)
C41 - C46 - C48 = 121.7(5)
C42 - C47 - H47A = 109.5
C42 - C47 - H47B = 109.5
H47A - C47 - H47B = 109.5
C42 - C47 - H47C = 109.5
H47A - C47 - H47C = 109.5
H47B - C47 - H47C = 109.5
C46 - C48 - H48A = 109.5
C46 - C48 - H48B = 109.5
H48A - C48 - H48B = 109.5
C46 - C48 - H48C = 109.5
H48A - C48 - H48C = 109.5

H48B - C48 - H48C = 109.5
O50 - C49 - C56 = 111.9(6)
O50 - C49 - C44 = 115.5(5)
C56 - C49 - C44 = 112.4(6)
O50 - C49 - C52 = 97.6(6)
C56 - C49 - C52 = 109.1(7)
C44 - C49 - C52 = 109.1(6)
C49 - O50 - C51 = 113.2(6)
O50 - C51 - H51A = 109.5
O50 - C51 - H51B = 109.5
H51A - C51 - H51B = 109.5
O50 - C51 - H51C = 109.5
H51A - C51 - H51C = 109.5
H51B - C51 - H51C = 109.5
F53 - C52 - F55 = 107.5(8)
F53 - C52 - F54 = 108.8(8)
F55 - C52 - F54 = 107.3(7)
F53 - C52 - C49 = 110.9(7)
F55 - C52 - C49 = 111.7(7)
F54 - C52 - C49 = 110.5(7)
F57 - C56 - F58 = 107.4(7)
F57 - C56 - F59 = 107.2(7)
F58 - C56 - F59 = 103.4(8)
F57 - C56 - C49 = 115.8(8)
F58 - C56 - C49 = 112.3(7)
F59 - C56 - C49 = 109.9(7)
C1 - Ru1 - C15 = 102.6(2)
C1 - Ru1 - O8 = 79.4(2)
C15 - Ru1 - O8 = 174.81(19)
C1 - Ru1 - Cl1 = 102.18(19)
C15 - Ru1 - Cl1 = 88.89(16)
O8 - Ru1 - Cl1 = 86.00(11)
C1 - Ru1 - Cl2 = 96.58(19)
C15 - Ru1 - Cl2 = 97.82(16)
O8 - Ru1 - Cl2 = 86.63(11)
Cl1 - Ru1 - Cl2 = 158.20(6)

Torsion angles [°]

Ru1 - C1 - C2 - C7 = -3.9(7)
Ru1 - C1 - C2 - C3 = 176.3(5)
C7 - C2 - C3 - C4 = -0.2(9)
C1 - C2 - C3 - C4 = 179.6(6)
C2 - C3 - C4 - C5 = -1.0(9)
C3 - C4 - C5 - C6 = 2.2(10)

C4 - C5 - C6 - C7 = -2.0(10)
C5 - C6 - C7 - O8 = 177.8(6)
C5 - C6 - C7 - C2 = 0.7(9)
C3 - C2 - C7 - O8 = -177.1(5)
C1 - C2 - C7 - O8 = 3.1(8)
C3 - C2 - C7 - C6 = 0.4(9)
C1 - C2 - C7 - C6 = -179.5(6)
C6 - C7 - O8 - C9 = 5.7(9)
C2 - C7 - O8 - C9 = -177.0(5)
C6 - C7 - O8 - Ru1 = -178.5(5)
C2 - C7 - O8 - Ru1 = -1.2(6)
C7 - O8 - C9 - C11 = -161.8(5)
Ru1 - O8 - C9 - C11 = 23.2(7)
C7 - O8 - C9 - C10 = 75.5(7)
Ru1 - O8 - C9 - C10 = -99.5(6)
N19 - C15 - N16 - C41 = 176.1(5)
Ru1 - C15 - N16 - C41 = -14.1(7)
N19 - C15 - N16 - C17 = 0.8(6)
Ru1 - C15 - N16 - C17 = 170.6(4)
C15 - N16 - C17 - C18 = -3.1(7)
C41 - N16 - C17 - C18 = -178.7(5)
N16 - C17 - C18 - N19 = 3.8(7)
N16 - C15 - N19 - C21 = -165.1(5)
Ru1 - C15 - N19 - C21 = 26.6(9)
N16 - C15 - N19 - C18 = 2.0(7)
Ru1 - C15 - N19 - C18 = -166.3(5)
C17 - C18 - N19 - C15 = -3.8(8)
C17 - C18 - N19 - C21 = 164.8(5)
C15 - N19 - C21 - C22 = 73.9(8)
C18 - N19 - C21 - C22 = -92.7(7)
C15 - N19 - C21 - C26 = -109.0(7)
C18 - N19 - C21 - C26 = 84.4(7)
C26 - C21 - C22 - C23 = -1.3(8)
N19 - C21 - C22 - C23 = 175.7(5)
C26 - C21 - C22 - C27 = -179.1(6)
N19 - C21 - C22 - C27 = -2.1(8)
C21 - C22 - C23 - C24 = -0.2(8)
C27 - C22 - C23 - C24 = 177.6(5)
C22 - C23 - C24 - C25 = 0.7(8)
C22 - C23 - C24 - C29 = -179.4(5)
C23 - C24 - C25 - C26 = 0.4(8)
C29 - C24 - C25 - C26 = -179.5(5)
C24 - C25 - C26 - C21 = -1.8(8)
C24 - C25 - C26 - C28 = 176.9(5)
C22 - C21 - C26 - C25 = 2.3(8)

N19	- C21	- C26	- C25	= -174.7(5)
C22	- C21	- C26	- C28	= -176.4(5)
N19	- C21	- C26	- C28	= 6.5(8)
C25	- C24	- C29	- O30	= -31.7(7)
C23	- C24	- C29	- O30	= 148.4(5)
C25	- C24	- C29	- C32	= -156.4(5)
C23	- C24	- C29	- C32	= 23.7(8)
C25	- C24	- C29	- C36	= 79.7(7)
C23	- C24	- C29	- C36	= -100.2(7)
C32	- C29	- O30	- C31	= 60.2(7)
C36	- C29	- O30	- C31	= 177.8(5)
C24	- C29	- O30	- C31	= -66.2(7)
O30	- C29	- C32	- F33	= 38.9(7)
C36	- C29	- C32	- F33	= -72.2(8)
C24	- C29	- C32	- F33	= 165.3(5)
O30	- C29	- C32	- F34	= -80.9(7)
C36	- C29	- C32	- F34	= 168.0(6)
C24	- C29	- C32	- F34	= 45.5(8)
O30	- C29	- C32	- F35	= 159.0(5)
C36	- C29	- C32	- F35	= 47.9(8)
C24	- C29	- C32	- F35	= -74.6(7)
O30	- C29	- C36	- F39	= 53.5(7)
C32	- C29	- C36	- F39	= 169.8(6)
C24	- C29	- C36	- F39	= -65.5(8)
O30	- C29	- C36	- F38	= -66.5(8)
C32	- C29	- C36	- F38	= 49.8(9)
C24	- C29	- C36	- F38	= 174.5(6)
O30	- C29	- C36	- F40	= 173.7(5)
C32	- C29	- C36	- F40	= -70.0(7)
C24	- C29	- C36	- F40	= 54.7(8)
C15	- N16	- C41	- C42	= 104.4(7)
C17	- N16	- C41	- C42	= -80.6(7)
C15	- N16	- C41	- C46	= -81.4(7)
C17	- N16	- C41	- C46	= 93.6(7)
C46	- C41	- C42	- C43	= 7.9(9)
N16	- C41	- C42	- C43	= -178.0(5)
C46	- C41	- C42	- C47	= -168.6(5)
N16	- C41	- C42	- C47	= 5.5(9)
C41	- C42	- C43	- C44	= -2.2(10)
C47	- C42	- C43	- C44	= 174.3(6)
C42	- C43	- C44	- C45	= -2.2(10)
C42	- C43	- C44	- C49	= 177.2(6)
C43	- C44	- C45	- C46	= 1.1(10)
C49	- C44	- C45	- C46	= -178.3(6)
C44	- C45	- C46	- C41	= 4.3(9)

C44 - C45 - C46 - C48 = -172.2(6)
C42 - C41 - C46 - C45 = -9.0(9)
N16 - C41 - C46 - C45 = 176.8(5)
C42 - C41 - C46 - C48 = 167.5(6)
N16 - C41 - C46 - C48 = -6.7(8)
C43 - C44 - C49 - O50 = 165.4(6)
C45 - C44 - C49 - O50 = -15.2(9)
C43 - C44 - C49 - C56 = 35.3(10)
C45 - C44 - C49 - C56 = -145.3(7)
C43 - C44 - C49 - C52 = -85.8(8)
C45 - C44 - C49 - C52 = 93.5(7)
C56 - C49 - O50 - C51 = 62.7(8)
C44 - C49 - O50 - C51 = -67.6(8)
C52 - C49 - O50 - C51 = 177.0(6)
O50 - C49 - C52 - F53 = 55.6(8)
C56 - C49 - C52 - F53 = 172.1(7)
C44 - C49 - C52 - F53 = -64.8(8)
O50 - C49 - C52 - F55 = -64.3(8)
C56 - C49 - C52 - F55 = 52.2(10)
C44 - C49 - C52 - F55 = 175.3(7)
O50 - C49 - C52 - F54 = 176.3(6)
C56 - C49 - C52 - F54 = -67.2(8)
C44 - C49 - C52 - F54 = 55.9(8)
O50 - C49 - C56 - F57 = 154.9(7)
C44 - C49 - C56 - F57 = -73.2(9)
C52 - C49 - C56 - F57 = 47.9(9)
O50 - C49 - C56 - F58 = 31.0(11)
C44 - C49 - C56 - F58 = 162.9(7)
C52 - C49 - C56 - F58 = -75.9(10)
O50 - C49 - C56 - F59 = -83.5(8)
C44 - C49 - C56 - F59 = 48.4(9)
C52 - C49 - C56 - F59 = 169.6(6)
C2 - C1 - Ru1 - C15 = 177.4(4)
C2 - C1 - Ru1 - O8 = 2.3(4)
C2 - C1 - Ru1 - Cl1 = 85.8(5)
C2 - C1 - Ru1 - Cl2 = -83.1(5)
N19 - C15 - Ru1 - C1 = -9.1(6)
N16 - C15 - Ru1 - C1 = -176.1(4)
N19 - C15 - Ru1 - O8 = 104(2)
N16 - C15 - Ru1 - O8 = -63(2)
N19 - C15 - Ru1 - Cl1 = 93.1(5)
N16 - C15 - Ru1 - Cl1 = -73.8(4)
N19 - C15 - Ru1 - Cl2 = -107.7(5)
N16 - C15 - Ru1 - Cl2 = 85.3(4)
C7 - O8 - Ru1 - C1 = -0.6(4)

C9	- O8	- Ru1	- C1	= 174.8(5)
C7	- O8	- Ru1	- C15	= -114(2)
C9	- O8	- Ru1	- C15	= 61(2)
C7	- O8	- Ru1	- Cl1	= -103.8(3)
C9	- O8	- Ru1	- Cl1	= 71.6(4)
C7	- O8	- Ru1	- Cl2	= 96.7(3)
C9	- O8	- Ru1	- Cl2	= -87.9(4)