ELECTRONIC SUPPORTING INFORMATION

Thioether-Based Anchimeric Assistance for Asymmetric Coordination Chemistry with Ruthenium(II) and Osmium(II)

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Contents:

1. Materials and Methods

All reactions were carried out under an atmosphere of argon and coordination chemistry was performed in the dark. Solvents were distilled under argon from calcium hydride (CH_3CN, DMF, CH_2Cl_2) or sodium/benzophenone (Et_2O, toluene). Absolute ethanol was used without further drying. [(η^6-C_6H_6)Ru(bpy)Cl]Cl (**1**),[1] [(η^6-C_6H_6)Os(bpy)Cl]Cl (**4**)[2] and chiral amino alcohols[3,4] were prepared according to published procedures. All other reagents were purchased from Acros, Aldrich or Alfa and used without further purification. Column chromatography was performed with silica gel (300-400 mesh). ^{1}H- and ^{13}C-NMR spectra were recorded on a Bruker Avance (300 MHz), a Bruker AM (400 MHz) or a Bruker AM (500 MHz) spectrometer at ambient temperature. NMR standards used are as follows: (^{1}H-NMR) CD_3CN = 1.94 ppm, $CDCl_3$ = 7.26 ppm. (^{13}C-NMR) CD_3CN = 1.32 ppm, $CDCl_3$ = 77.00 ppm. ^{1}H NMR data are reported as follows: chemical shift in ppm downfield from tetramethylsilane (δ scale), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, and br = broad), coupling constant (Hz), and integration. ^{13}C NMR chemical shifts are reported in ppm downfield from tetramethylsilane (δ scale). IR spectra were recorded on a Nicolet Avatar 330 RT-IR spectrophotometer. Chiral HPLC chromatograms were obtained from an Agilent 1260 Series HPLC system. CD spectra were recorded on a JASCO J-810 CD spectropolarimeter (200-600 nm, band width of 1 nm, scanning speed of 50 nm/min, accumulation of 3 scans). High-resolution mass spectra were recorded on a Bruker Apex Ultra FTMS 7.0 T instrument using ESI technique.

2. Synthesis of Chiral Ligands

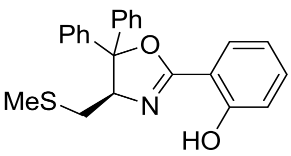
2.1. Synthesis of amino alcohols

The amino alcohol (*R*)-2-amino-1,1-diphenyl-3-methylthio-1-propanol was synthesized according to published procedures.[3] The remaining amino alcohols were synthesized according to the following procedure:[4] A solution of amino acid methyl ester or its hydrochloride (1 eq) in dry diethyl ether (0.4 M) was added dropwise to a stirred solution of freshly prepared methyl magnesium iodide (4 or 6 eq). The reaction mixture was refluxed for 1-2 hours and then quenched with aqueous ammonium chloride. The organic layer was separated and the aqueous phase was extracted three times with diethyl ether. The combined organic phase was dried over anhydrous sodium sulfate, then dried under high vacuum and the obtained products were used directly for the next step without further purification.

2.2. Synthesis of 2-(2'-hydroxyphenyl)oxazoline derivatives

The oxazolines (*S*)-4-isopropyl-2-(2'-hydroxyphenyl)-2-oxazoline (**2a**), (*R*)-4-(methylthiomethyl)-2-(2'-hydroxyphenyl)-2-oxazoline (**2b**), (*R*)-5,5-dimethyl-4-(methylthio methyl)-2-(2'-hydroxyphenyl)-2-oxazoline (**2d**), and (*S*)-4-(methylthioethyl)-2-(2'-hydroxyphenyl)-2-oxazoline (**2h**) were synthesized following published procedures.[4,5] The derivatives (*R*)-5,5-diphenyl-4-(methylthiomethyl)-2-(2'-hydroxyphenyl)-2-oxazoline (**2c**), (*R*)-5,5-dimethyl-4-(isopropylthiomethyl)-2-(2'-hydroxyphenyl)-2-oxazoline (**2e**), (*R*)-5,5-dimethyl-4-(*tert*-butylthiomethyl)-2-(2'-hydroxyphenyl)-2-oxazoline (**2f**), and the auxiliary (*R*)-5-(benzylthiomethyl)-4,4-dimethyl-2-(2'-hydroxyphenyl)-2-oxazoline (**2g**) were synthesized with modifications of a published procedure[4] as follows: Amino alcohol (1.0 eq), 2-hydroxylbenzonitrile (1.2 eq), and zinc chloride (0.020 eq) were dissolved in toluene (1.0 M) under argon. The mixture was heated at reflux for 24 h and afterwards dried under vacuum to give an oily residue which was redissolved in dichloromethane and washed with water. The organic phase was separated and dried over anhydrous sodium sulfate. After filtration and evaporation, the crude product was purified by silica gel column chromatography.

(R)-5,5-Diphenyl-4-(methylthiomethyl)-2-(2'-hydroxyphenyl)-2-oxazoline (2c)



Synthesized from (*R*)-2-amino-1,1-diphenyl-3-methylthio-l-propanol as described above.[3] The crude material was purified by silica gel column chromatography (elution with hexanes/EtOAc = 20: 1) to give the pure product as a white solid. Yield: 51%.

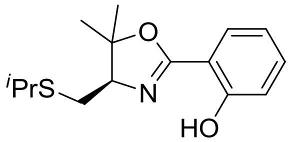
^{1}H-NMR (300.1 MHz, $CDCl_3$): δ (ppm) 11.90 (br, 1H), 7.83 (dd, J = 7.8, 1.5 Hz, 1H), 7.52 (m, 2H), 7.25 (m, 9H), 6.96 (dd, J = 8.4, 0.6 Hz, 1H), 6.86 (td, J = 7.2, 1.2 Hz, 1H), 5.06 (dd, J = 8.4, 5.7 Hz, 1H), 2.30 (m, 2H), 2.05 (s, 3H).

^{13}C-NMR (75.5 MHz, $CDCl_3$): δ (ppm) 164.2, 160.2, 143.0, 139.3, 136.5, 133.8, 129.0, 128.6, 128.4, 128.3, 128.2, 128.0, 126.8, 126.5, 120.1, 119.0, 118.8, 117.0, 110.5, 92.5, 74.5, 38.2, 16.8.

IR (neat): ν (cm^{-1}) 3059, 2921, 2798, 2642, 1646, 1620, 1582, 1535, 1489, 1448, 1427, 1412, 1357, 1310, 1285, 1258, 1237, 1189, 1156, 1137, 1102, 1079, 1035, 999, 969, 936, 924, 897, 829, 791, 752, 700, 630, 529.

HRMS calcd for $C_{23}H_{21}SO_2NNa$ $(M+Na)^+$ 398.1185, found: 398.1185.

(R)-5,5-Dimethyl-4-(isopropylthiomethyl)-2-(2'-hydroxyphenyl)-2-oxazoline (2e)



Synthesized from (*R*)-2-amino-1,1-dimethyl-3-isopropylthio-l-propanol as described above. The crude material was purified by column chromatography (elution with hexanes/EtOAc = 50: 1) to give the pure product as a brownish yellow oil. Yield: 68%.

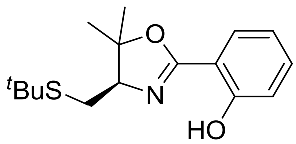
^{1}H-NMR (400.1 MHz, $CDCl_3$) δ (ppm) 12.21 (br, 1H), 7.61 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.35 (m, 1H), 6.99 (dd, *J* = 8.3, 0.8 Hz, 1H), 6.84 (m, 1H), 4.06 (dd, *J* = 8.5, 6.0 Hz, 1H), 3.04 (hept, *J* = 6.7 Hz, 1H), 2.90 (dd, *J* = 13.1, 6.0 Hz, 1H), 2.68 (dd, *J* = 13.1, 8.5 Hz, 1H), 1.58 (s, 3H), 1.44 (s, 3H), 1.32 (d, *J* = 1.6 Hz, 3H), 1.30 (d, *J* = 1.6 Hz, 3H).

^{13}C-NMR (100.6 MHz, $CDCl_3$) δ (ppm) 164.4, 160.1, 133.3, 128.1, 118.5, 116.8, 110.9, 86.2, 73.3, 35.9, 31.6, 29.70, 28.8, 23.5, 21.5.

IR (film): ν (cm^{-1}) 3064, 2961, 2926, 2866, 1638, 1616, 1490, 1457, 1419, 1386, 1364, 1342, 1312, 1261, 1237, 1153, 1124, 1068, 1034, 967, 848, 799, 756, 686.

HRMS calcd for $C_{15}H_{22}NO_2S$ $(M+H)^+$ 280.1366, found: 280.1369.

(R)-5,5-Dimethyl-4-(tert-butylthiomethyl)-2-(2'-hydroxyphenyl)-2-oxazoline (2f)



Synthesized from (*R*)-2-amino-1,1-dimethyl-3-*tert*-butylthio-l-propanol as described above. The crude product was purified by column chromatography (elution with hexanes/EtOAc = 30: 1) to give the pure product as a brownish yellow oil. Yield: 76%.

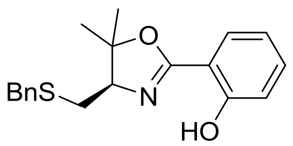
^{1}H-NMR (400.1 MHz, $CDCl_3$) δ (ppm) 12.22 (br, 1H), 7.61 (dd, J = 7.8, 1.7 Hz, 1H), 7.35 (m, 1H), 6.99 (dd, J = 8.3, 0.8 Hz, 1H), 6.85 (td, J = 7.8, 1.0 Hz, 1H), 4.03 (dd, J = 9.5, 5.3 Hz, 1H), 2.92 (dd, J = 12.4, 5.3 Hz, 1H), 2.69 (dd, J = 12.4, 9.5 Hz, 1H), 1.57 (s, 3H), 1.45 (s, 3H), 1.36 (s, 9H).

^{13}C-NMR (100.1MHz, $CDCl_3$) δ (ppm) 164.3, 160.1, 133.3, 128.1, 118.5, 116.8, 110.9, 86.3, 73.2, 42.7, 30.8, 29.4, 28.8, 21.5.

IR (film): ν (cm^{-1}) 3061, 2959, 2923, 2849, 1641, 1615, 1582, 1536, 1491, 1460, 1386, 1364, 1342, 1312, 1261, 1237, 1153, 1123, 1068, 1034, 961, 848, 799, 755, 686.

HRMS calcd for $C_{16}H_{24}NO_2S$ $(M+H)^+$ 294.1522, found: 294.1526.

(R)-4-(Benzylthiomethyl)-5,5-dimethyl-2-(2'-hydroxyphenyl)-2-oxazoline (2g)



Synthesized from (*R*)-2-amino-1,1-dimethyl-3-benzylthio-l-propanol as described above. The crude product was purified by silica gel column chromatography (elution with hexanes/EtOAc = 50: 1) to give the pure product as a pale yellow oil. Yield: 71%.

^{1}H-NMR (400.1 MHz, $CDCl_3$): δ (ppm) 12.21 (br, 1H), 7.59 (dt, J = 10.6, 5.3 Hz, 1H), 7.33 (m, 5H), 7.24 (m, 1H), 6.98 (d, J = 8.3 Hz, 1H), 6.84 (t, J = 7.5 Hz, 1H), 3.97 (dd, J = 7.9, 6.5 Hz, 1H), 3.81 (s, 2H), 2.76 (dd, J = 13.3, 6.3 Hz, 1H), 2.58 (dd, J = 13.3, 8.1 Hz, 1H), 1.50 (s, 3H), 1.35 (s, 3H).

^{13}C-NMR (100.6 MHz, $CDCl_3$): δ (ppm) 164.6, 160.2, 138.2, 133.5, 129.1, 128.7, 128.2, 127.3, 118.6, 116.9, 111.0, 86.2, 72.7, 37.4, 32.5, 28.8, 21.6.

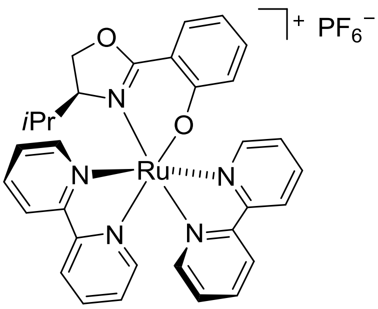
IR (film): *ν* (cm^{-1}) 3061, 3027, 2974, 2921, 1637, 1615, 1582, 1492, 1453, 1422, 1386, 1364, 1343, 1312, 1260, 1238, 1153, 1124, 1069, 1033, 805, 756, 701.

HRMS calcd for $C_{19}H_{22}NO_2S$ $(M+H)^+$ 328.1366, found: 328.1370.

3. Diastereoselective Synthesis of Ruthenium and Osmium Complexes

General method for the diastereoselective synthesis of ruthenium complexes according to Table 1: A mixture of [(η^6-C_6H_6)Ru(bpy)Cl]Cl (**1**)[1] (15.0 mg, 0.037 mmol, 1.0 eq), chiral oxazoline (1.1 eq), 2,2'-bipyridine (6.9 mg, 0.044 mmol, 1.2 eq), and triethylamine (53.4 µL, 0.37 mmol, 10 eq) in ethanol (15 mL, 2.5 mM) was heated at reflux under argon overnight in the dark. The solvent was then removed under reduced pressure and the residue was purified by silica gel column chromatography (CH_3CN: H_2O: KNO_3 (sat) = 100: 3: 1). The eluents were concentrated to dryness and the resulting material dissolved in minimal amounts of ethanol/water. The product was precipitated by the addition of excess solid NH_4PF_6. The precipitate was centrifuged, washed twice with water, and dried under high vacuum to afford a brownish or purple solid.

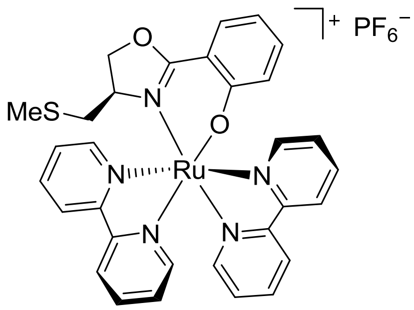
Ruthenium complex Λ-3a [5]



Synthesized with the chiral oxazoline **2a** (13.4 mg, 0.041 mmol). The crude material was purified by silica gel column chromatography (CH_3CN: H_2O: KNO_3(sat) = 100: 3: 1) to give a brownish purple product with a diastereomeric ratio of Δ:Λ = 1:2 which was determined by ^{1}H-NMR. Yield: 7.6 mg (27%). The metal-centered configuration was assigned by CD spectroscopy (Figure S1).[5]

CD (MeCN): λ, nm (Δε, $M^{-1}cm^{-1}$) 285 (-18), 299 nm (+56).

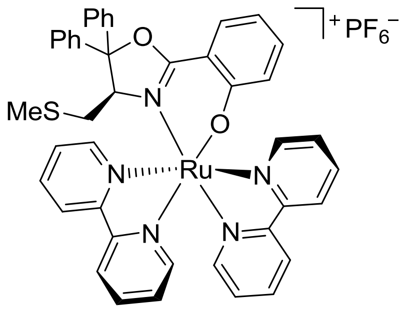
Ruthenium complex Δ-3b[6]



Synthesized with the chiral oxazoline **2b** (10.3 mg, 0.041 mmol). The crude material was purified by silica gel column chromatography (CH_3CN: H_2O: KNO_3(sat) = 100: 3: 1) to give a brownish purple product with a diastereomeric ratio of Δ:Λ = 11:1 which was determined by ^{1}H-NMR. Yield: 19.5 mg (61%). The metal-centered configuration was assigned by CD spectroscopy (Figure S2).[6]

CD (MeCN): λ, nm (Δε, $M^{-1}cm^{-1}$) 299 (-101), 364 (+12).

Ruthenium complex Δ-3c



Synthesized with the chiral oxazoline **2c** (15.4 mg, 0.041mmol). The crude material was purified by silica gel column chromatography (CH_3CN: H_2O: KNO_3 (sat) = 150: 3: 1) to give a brownish purple product with a diastereomeric ratio of 19:1 which was determined by ^{1}H NMR. Yield: 21.3 mg, 59%. The metal-centered configuration was assigned by CD spectroscopy (Figure S3).

^{1}H-NMR (500.1 MHz, CD_3CN) for the major diastereomer: δ (ppm) 9.25 (d, J = 5.5 Hz, 1H), 8.46 (dd, J = 8.0 Hz, 1H), 8.42 (dd, J = 8.0 Hz, 2H), 8.36 (d, J = 8.0 Hz, 1H), 8.26 (d, J = 5.5, 1H), 8.02

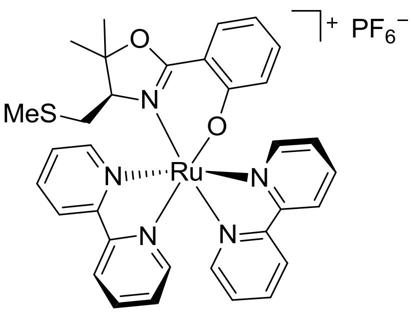
(td, *J* = 7.9, 1.3 Hz, 1H), 7.99 (m, 2H), 7.87 (td, *J* = 7.9, 1.3 Hz, 1H), 7.82 (m, 2H), 7.54 (ddd, *J* = 7.1, 5.7, 1.1 Hz, 1H), 7.48 (m, 2H), 7.44 (d, *J* = 5.6 Hz, 1H), 7.29 (m, 4H), 7.18 (t, *J* = 8.0 Hz, 1H), 7.08 (m, 6H), 6.50 (t, *J* = 7.5 Hz, 1H), 5.32 (d, *J* = 8.6 Hz, 1H), 3.63 (dd, *J* = 8.6, 2.7 Hz, 1H), 2.64 (m, 2H), 1.34 (s, 3H).

^{13}C-NMR (125.8 MHz, CD_3CN) for the major diastereomer: δ (ppm) 170.2, 161.9, 159.4, 158.2, 157.9, 157.1, 154.1, 152.8, 151.3, 149.8, 142.8, 138.9, 136.4, 136.0, 135.8, 134.9, 133.0, 129.6, 129.4, 128.7, 128.03, 127.99, 127.8, 127.3, 126.5, 126.4, 125.73, 125.70. 125.4, 113.3, 110.3, 91.7, 73.3, 35.8, 15.3.

IR (neat): ν (cm^{-1}) 3060, 2962, 2922, 1611, 1536, 1493, 1467, 1443, 1420, 1378, 1350, 1260, 1240, 1191, 1157, 1078, 1019, 928, 875, 837, 799, 758, 730, 701, 658, 592, 557. HRMS calcd for $C_{43}H_{36}RuSO_2N_5$ $(M-PF_6)^+$ 788.1639, found: 788.1639.

CD (MeCN): λ, nm (Δε, $M^{-1}cm^{-1}$) 300 (-76), 285 (+21)

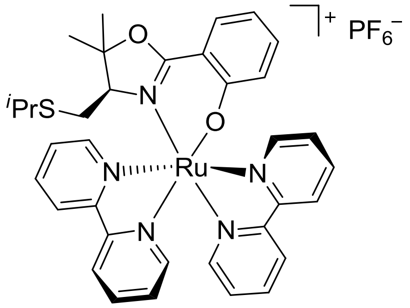
Ruthenium complex Δ-3d[6]



Synthesized with the chiral oxazoline **2d** was used (8.4 mg, 0.041 mmol). The crude material was purified by silica gel column chromatography (CH_3CN: H_2O: KNO_3(sat) = 100: 3: 1) to give a brownish purple product with a diastereomeric ratio of 22:1 which was determined by ^{1}H-NMR. Yield: 22.1 mg (74%). The metal-centered configuration was assigned by CD spectroscropy (Figure

S4).[6] CD (MeCN): λ, nm (Δε, $M^{-1}cm^{-1}$) 298 (-85), 364 (+17).

Ruthenium complex Δ-3e



Synthesized with the chiral oxazoline **2e** (11.5 mg, 0.041 mmol). The crude material was purified by silica gel column chromatography (CH_3CN: H_2O: KNO_3(sat) = 100: 3: 1) to give a brownish purple product with a diastereomeric ratio of 16:1 as determined by ^{1}H-NMR. Yield: 23.1 mg (71%). The relative metal-centered configuration was assigned by CD spectroscopy (Figure S5) .

^{1}H-NMR (400.1 MHz, CD_3CN) for the major diastereomer: δ (ppm) 9.07 (d, *J* = 5.6, 1H), 8.82 (d, *J* = 5.6, 1H), 8.48 (d, *J* = 8.1 Hz, 1H), 8.44 (d, *J* = 8.0 Hz, 1H), 8.36 (d, *J* = 8.1 Hz, 2H), 8.08 (ddd, *J* = 9.3, 5.8, 1.5 Hz, 1H), 7.97 (td, *J* = 7.9 Hz, 1.4 Hz, 1H), 7.93 (d, *J* = 5.7, 1H), 7.83 (td, *J* = 8.0 Hz, 1.4 Hz, 1H), 7.77 (td, *J* = 8.0 Hz, 1.4 Hz, 1H), 7.63 (m, 2H), 7.49 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.43 (m, 1H), 7.11 (m, 2H), 6.98 (ddd, *J* = 8.7, 6.9, 1.9 Hz, 1H), 6.33 (m, 2H), 2.73 (dd, *J* = 12.1, 10.5 Hz, 1H), 2.43 (m, 3H), 1.52 (s, 3H), 1.08 (d, *J* = 6.7 Hz, 3H), 1.01 (d, *J* = 6.7 Hz, 3H), 0.59 (s, 3H).

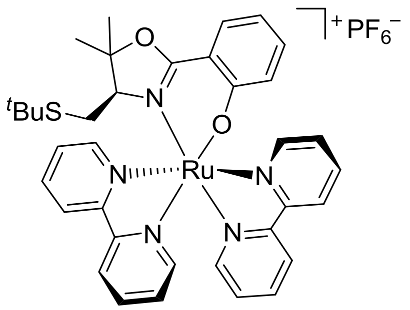
^{13}C-NMR (100.6 MHz, CD_3CN) for the major diastereomer: δ (ppm) 171.1, 162.9, 160.4, 159.2, 158.9, 158.9, 154.8, 153.6, 152.5, 151.6 137.1, 136.9, 136.7, 135.6, 133.6, 130.5, 127.8, 127.4, 126.7, 126.4, 124.9, 124.3, 124.2, 124.1, 123.9, 113.9, 111.6, 86.1, 73.2, 37.6, 32.3, 28.2, 23.9, 23.6, 21.4.

IR (film): ν (cm^{-1}) 3367, 2963, 2923, 2845, 1611, 1534, 1450, 1384, 1259, 1195, 1155, 1086, 1052, 869, 845, 799, 747, 607, 543.

HRMS calcd for $C_{35}H_{36}N_5O_2RuS$ $(M-PF_6)^+$ 692.1633, found: 692.1616.

CD (MeCN): λ, nm (Δε, $M^{-1}cm^{-1}$) 301 (-56), 366 (+11).

Ruthenium complex Δ-3f



Synthesized with the chiral oxazoline **2f** (12.0 mg, 0.041 mmol). The crude material was purified by silica gel column chromatography (CH_3CN: H_2O: KNO_3(sat) = 100: 3: 1) to give a brownish purple product with a diasteremeric ratio of 8:1 as determined by ^{1}H-NMR. Yield: 25.5 mg, 67%. The metal-centered configuration was assigned by CD spectroscopy (Figure S6).

^{1}H-NMR (400.1 MHz, CD_3CN) for the major diastereomer: δ (ppm) 9.12 (d, J = 5.6, , 1H), 8.85 (d, J = 5.7 Hz, 1H), 8.48 (m, 2H), 8.38 (m, 2H), 8.09 (td, J = 7.7, 1.5 Hz, 1H), 7.98 (td, J = 7.9, 1.5 Hz, 1H), 7.87 (d, J = 5.7 Hz, 1H), 7.83 (td, J = 7.8, 1.5 Hz, 1H), 7.76 (td, J = 7.9, 1.5 Hz, 1H), 7.62 (m, 2H), 7.52 (dd, J = 8.1, 1.8 Hz, 1H), 7.46 (m, 1H), 7.12 (m, 2H), 7.01 (ddd, J = 8.7, 6.9, 1.9 Hz, 1H), 6.35 (m, 2H), 2.73 (t, J = 10.8 Hz, 1H), 2.55 (dd, J = 11.0, 1.6 Hz, 1H), 2.38 (dd, J = 10.5, 1.6 Hz, 1H), 1.59 (s, 3H), 1.16 (s, 9H), 0.61 (s, 3H).

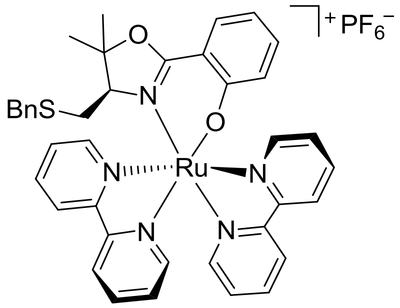
^{13}C-NMR (100.1 MHz, CD_3CN) for the major diastereomer: δ (ppm) 171.0, 162.8, 160.2, 159.1, 159.0, 158.9, 154.7, 153.6, 152.6, 151.6, 137.0, 136.9, 136.7, 135.6, 133.6, 130.5, 127.8, 127.6, 126.7, 126.4, 124.8, 124.4, 124.3, 124.1, 123.9, 113.8, 111.5, 86.3, 71.9, 42.9, 30.8, 29.4, 28.3, 21.3.

IR (film): *ν* (cm^{-1}) 3385, 2960, 2924, 2851, 1661, 1650, 1609, 1534, 1468, 1442, 1412, 1384, 1342, 1246, 1153, 1069, 1043, 872, 766, 729, 656, 650, 543.

HRMS calcd for $C_{36}H_{38}N_5O_2RuS$ $(M\text{-}PF_6)^+$, 706.1790, found: 706.1798.

CD (MeCN): λ, nm (Δε, $M^{-1}cm^{-1}$) 301 (-37), 359 (+9).

Ruthenium complex Δ-3g



Synthesized with the chiral oxazoline **2g** (13.4 mg, 0.041 mmol). The crude material was purified by silica gel column chromatography (CH_3CN: H_2O: KNO_3(sat) = 150: 3: 1) to give a brownish purple product with a diastereomeric ratio of 24:1 as determined by ^{1}H-NMR. Yield: 26.8 mg (82%). The product purity could be further improved by precipitation from CH_2Cl_2/Et_2O. For this, Δ-**3g** was first dissolved in CH_2Cl_2 (2 mL), then Et_2O (6 mL) was added slowly under stirring, and the formed precipitation was centrifuged and dried under high vacuum to give the product with d.r. > 100:1. Yield: 23.1 mg (86%). The metal-centered configuration was assigned by CD spectroscopy (Figure S7) and confirmed by X-ray crystallography (Figure S18).

^{1}H-NMR (400.1 MHz, CD_3CN) for the major diastereomer: δ (ppm) 8.95 (d, *J* = 5.2 Hz, 1H), 8.78 (d, *J* = 5.2, 1H), 8.45 (dd, *J* = 11.6, 8.2 Hz, 2H), 8.33 (t, *J* = 7.6 Hz, 2H), 8.06 (td, *J* = 8.0, 1.5 Hz, 1H), 8.01 (td, *J* = 8.0, 1.4 Hz, 1H), 7.80 (td, *J* = 8.0, 1.4 Hz, 1H), 7.71 (td, *J* = 8.0, 1.3 Hz, 1H), 7.59 (m, 2H), 7.48 (ddd, *J* = 8.7, 6.5, 1.5 Hz, 3H), 7.21 (m, 3H), 7.11 (m, 3H), 6.98 (ddd, *J* = 8.7, 6.9, 1.9 Hz, 1H), 6.87 (ddd, *J* = 7.2, 5.7, 1.2 Hz, 1H), 6.35 (m, 2H), 3.40 (m, 2H), 2.65 (dd, *J* = 11.9, 10.9 Hz, 1H), 2.42 (m, 2H), 1.49 (s, 3H), 0.56 (s, 3H).

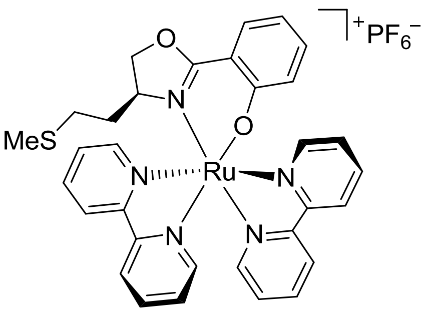
^{13}C-NMR (100.6 MHz, CD_3CN) for the major diastereomer: δ (ppm) 171.1, 162.99, 160.3, 159.1, 159.0, 158.9, 154.4, 153.6, 152.5, 151.6, 139.1, 137.1, 136.9, 136.7, 135.5, 133.7, 130.6, 129.9, 129.5, 128.1, 127.8, 127.6, 126.8, 124.9, 124.4, 124.2, 123.9, 113.9, 111.4, 86.2, 72.6, 37.7, 33.5, 28.0, 21.4.

IR (film): ν (cm^{-1}) 3397, 2921, 2848, 1667, 1609, 1536, 1469, 1442, 1418, 1390, 1349, 1247, 1155, 1069, 1019, 873, 839, 763, 730, 706, 558.

HRMS calcd for $C_{39}H_{36}N_5O_2RuS$ $(M\text{-}PF_6)^+$ 740.1633, found: 740.1628.

CD (MeCN): λ, nm (Δε, $M^{-1}cm^{-1}$) 301 (-103), 285(+21).

Ruthenium complex Δ-3h



Synthesized with the chiral oxazoline **2h** (9.7 mg, 0.041 mmol). The crude material was purified by silica gel column chromatography (CH_3CN: H_2O: KNO_3(sat) = 100: 3: 1) to give a brownish purple product with a diastereomeric ratio of 2.3:1 as determined by ^{1}H-NMR. Yield: 9.1 mg (31%). The metal-centered configuration was assigned by CD spectroscopy (Figure S8).

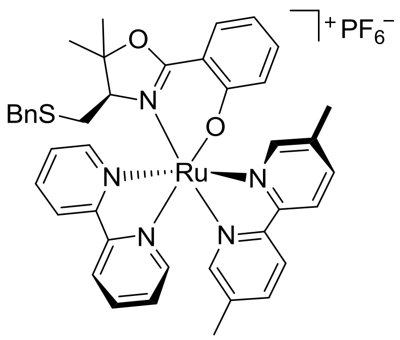
^{1}H-NMR (300.1 MHz, CD_3CN) for the major diastereomer: δ (ppm) 8.96 (dq, J = 5.7, 0.6 Hz, 1H), 8.81 (m, 1H), 8.50 (d, J = 8.1 Hz, 1H), 8.46 (d, J = 8.1 Hz, 1H), 8.09 (td, J = 7.8, 1.5 Hz, 1H), 7.54-8.02 (m, 9 H), 7.47 (ddd, J = 7.2, 5.7, 1.2 Hz, 1H), 7.16 (m, 1H), 7.09 (ddd, J = 7.2, 5.7, 1.2 Hz, 1H), 7.02 (m, 1H), 6.37 (m, 2 H), 4.26 (dd, J = 9.0, 4.5 Hz, 1H), 4.03 (t, J = 9.0 Hz, 1H), 2.95 (m, 1H), 1.88 (s, 3H), 1.74-2.02 (m, 4H).

IR (film): ν (cm^{-1}) 3072, 2971, 2912, 1606, 1536, 1461, 1442, 1418, 1387, 1346, 1309, 1260, 1233, 1156, 1074, 1035, 1018, 978, 930, 878, 830, 756, 727, 686, 656, 576.

HRMS calcd for $C_{32}H_{30}RuSO_2N_5$ $(M-PF_6)^+$ 650.1166, found: 650.1160.

CD (MeCN): λ, nm ($\Delta\varepsilon$, $M^{-1}cm^{-1}$) 299 (-17), 363 (+8).

Synthesis of Δ-[Ru(bpy)(dmb)(2g-H)]PF$_6$



A mixture of [(η^6-C_6H_6)Ru(bpy)Cl]Cl (**1**) (15.0 mg, 0.037 mmol), chiral oxazoline **2g** (13.4 mg), 5,5'-dimethyl-2,2'-bipyridine (8.2 mg, 0.044 mmol), and triethylamine (53.4 µL, 0.37 mmol, 10 eq) in ethanol (15 mL, 2.5 mM) was heated at reflux under argon overnight. The solvent was then removed under reduced pressure and the residue was purified by column chromatography (CH_3CN: H_2O: KNO_3 (sat) = 150: 3: 1). The eluents were concentrated to dryness and the resulting material was dissolved in minimal amounts of ethanol/water. The product was precipitated by the addition of excess solid NH_4PF_6. The precipitate was centrifuged, washed twice with water, and dried under high vacuum to afford a brownish solid as a 4:1 mixture of two Δ-diastereomers. Yield: 27.4 mg (81%). The absolute metal-centered configuration was assigned by CD spectroscopy (Figure S9).

^{1}H-NMR (400.1 MHz, CD_3CN) for the major diastereomer: δ (ppm) 8.99 (d, J = 5.4 Hz, 1H), 8.59 (s, 1H), 8.43 (d, J = 8.0 Hz, 1H), 8.35 (d, J = 8.1 Hz, 1H), 8.31 (d, J = 8.3 Hz, 1H), 8.19 (d, J = 8.3 Hz, 1H), 7.97 (td, J = 8.0, 1.3 Hz, 1H), 7.88 (dd, J = 8.3, 1.2 Hz, 1H), 7.82 (td, J = 8.0, 1.3 Hz, 1H), 7.69 (s, 1H), 7.60 (d, J = 5.0 Hz, 1H), 7.56 (dd, J = 8.3, 0.96 Hz, 1H), 7.46 (dd, J = 8.1, 1.8 Hz, 1H), 7.41 (m, 1H), 7.28 (d, J = 7.5 Hz, 1H), 7.23 (m, 2H), 7.15 (m, 2H), 7.11 (m, 1H), 6.96 (ddd, J = 8.7, 6.9, 1.9 Hz, 1H), 6.34 (m, 1H), 6.28 (d, J = 8.6 Hz, 1H), 3.32 (m, 2H), 2.66 (m, 1H), 2.52 (m, 2H), 2.36 (s, 3H), 2.04 (s, 3H), 1.43 (s, 3H), 0.59 (s, 3H).

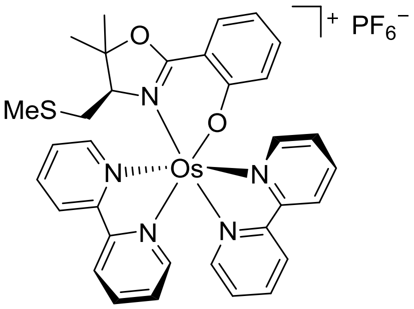
^{13}C-NMR (100.6 MHz, CD_3CN) for the major diastereomer: δ (ppm) 171.1, 163.1, 159.4, 159.0, 157.9, 156.4, 154.5, 153.7, 152.5, 151.2, 139.1, 138.3, 137.9, 137.7, 136.6, 136.6, 136.5, 133.6, 130.5, 129.7, 129.6, 129.6, 129.5, 128.1, 128.1, 126.5, 126.5, 124.3, 124.1, 123.9, 123.3 , 113.8, 86.2, 72.7, 37.9, 33.9, 27.9, 21.4, 18.8, 18.3.

IR (film): ν (cm^{-1}) 3072, 2971, 2912, 1606, 1536, 1461, 1442, 1418, 1387, 1346, 1309, 1260, 1233, 1156, 1074, 1035, 1018, 978, 930, 878, 830, 756, 727, 686, 656, 576.

HRMS calcd for $C_{41}H_{40}N_5O_2RuS$ $(M-PF_6)^+$ 768.1946, found: 768.1935.

CD (MeCN): λ, nm (Δε, $M^{-1}cm^{-1}$) 304 (-104), 289 (+27).

Synthesis of osmium complex Δ-5



A mixture of [(η^6-C_6H_6)Os(bpy)Cl]Cl (**4**)[2] (165.3 mg, 0.334 mmol, 1.0 eq), chiral oxazoline **2d** (94.5 mg, 0.376mmol, 1.1 eq), 2,2'-bipyridine (63.3 mg, 0.401 mmol, 1.2 eq), and K_2CO_3 (468.4 mg, 3.36 mmol, 10 eq) in ethylene glycol (3.4 mL, 100 mM) was heated at 150 °C for 3 h under argon. The reaction mixture was cool down, into which NH_4PF_6 (220 mg, 1.35 mmol, 4 eq) in 9 mL of H_2O was added to precipitate the crude product as PF_6 salt. The dark-brown precipitation was collected by centrifugation, washed with cold water, dried under high vacuum, and then subjected to silica gel chromatography (CH_2Cl_2: acetone: aqueous ammonia = 7 : 1: 0.005). The eluents were concentrated to dryness and washed by ether to afford the product with a diastereomer ratio (Δ:Λ) of 11:1 as determined by ^{1}H NMR (Yield: 158 mg, 53%). The pure diastereomer Δ-**5** could be obtained by an additional precipitation of a acetone solution of Δ-**5** with Et_2O (ratio acetone:Et_2O = 7 : 1, volume 8 mL). Overall yield: 117 mg (39.0%). The metal-centered configuration was assigned by CD spectroscopy (Figure S10) and confirmed by X-ray crystallography (Figure S19).

^{1}H-NMR (400.1 MHz, acetone-d_6) for the major diastereomer: δ (ppm) 9.06 (d, J = 6.0 Hz, 1H), 8.79 (d, J = 8.4 Hz, 1H), 8.71 (d, J = 6.0 Hz, 1H), 8.66 (d, J = 8.0 Hz, 1H), 8.60 (d, J = 8.0 Hz, 1H), 8.56 (d, J = 8.4 Hz, 1H), 8.14 (d, J = 5.6 Hz, 1H), 7.89 (t, J = 8.0 Hz, 1H), 7.68 (m, 3H), 7.55 (m, 2H), 7.49 (d, J = 5.6 Hz, 1H), 7.36 (t, J = 6.4 Hz, 1H), 7.07 (m, 3H), 6.43 (t, J = 7.6 Hz, 1H), 6.38

(d, *J* = 8.8 Hz, 1H), 2.97 (dd, *J* = 12.4, 10.8 Hz, 1H), 2.68 (d, *J* = 10.8 Hz, 1H), 2.64 (d, *J* = 12.4 Hz, 1H), 1.71 (s, 3H), 1.53 (s, 3H), 0.76 (s, 3H).

^{13}C-NMR (100.6 MHz, acetone-d_6) for the major diastereomer: δ (ppm) 167.6, 163.6, 161.4, 161.1, 160.0, 158.6, 154.0, 151.3, 150.3, 148.6, 136.0, 134.9, 134.6, 132.8, 132.1, 128.8, 127.8, 127.3, 126.0, 125.9, 124.6, 123.4, 123.1, 123.0, 122.9, 114.1, 110.9, 85.5, 72.1, 34.0, 27.2, 20.6, 15.0.

IR (film): ν (cm^{-1}) 3061, 2963, 2912, 2851, 1606, 1584, 1537, 1458, 1470, 1441, 1417, 1393, 1256, 1154, 1074, 1016, 839, 799, 724, 659, 557.

HRMS calcd for $C_{35}H_{32}N_5O_2OsS$ $(M-PF_6)^+$ 754.1892, found: 754.1906.

CD (MeOH): λ, nm (Δε, $M^{-1}cm^{-1}$) 301 (-51), 275 (+22).

4. TFA-Induced Removal of Chiral Auxiliaries

Synthesis of Δ-[Ru(bpy)$_3$](PF$_6$)$_2$

In a sealed brown glass vial fitted with a septum, a solution of Δ-**3g** (8.9 mg, 0.010 mmol) and 2,2'-bipyridine (23.4 mg, 0.150 mmol) in CH_3CN (0.2 mL) was heated at 110 °C (oil bath temperature) for 2 h under argon atmosphere. The reaction mixture was cooled to room temperature and dried in vacuo. The crude material was subjected to silica gel chromatography with acetonitrile and later CH_3CN: H_2O: KNO_3(sat) = 50 : 6 : 2. The product eluents were concentrated to dryness, the resulting material was dissolved in minimal amounts of ethanol/water, and the product was precipitated by the addition of excess solid NH_4PF_6. The orange precipitate was centrifuged, washed twice with water, and dried under high vacuum to afford Δ-[Ru(bpy)$_3$](PF$_6$)$_2$ (7.8 mg, 91%). The enantiopurity (100:1 e.r.) of the product was determined by chiral HPLC analysis (Figure S14).

Synthesis of Δ-[Ru(bpy)(dmb)(phen)](PF$_6$)$_2$

In a sealed brown glass vial fitted with a septum, a solution of Δ-[Ru(bpy)(dmb)(**2g**-H)]PF$_6$ (9.2 mg, 0.010 mmol), trifluoroacetic acid (3.7 μL, 0.050 mmol) and 1,10-phenanthroline (27.0 mg, 0.15 mmol) in CH_3CN (0.2 mL) was heated at 110 °C (oil bath temperature) for 2 h under argon atmosphere. The reaction mixture was cooled to room temperature and dried in vacuo. The crude material was subjected to silica gel chromatography with acetonitrile and later CH_3CN: H_2O: KNO_3(sat) = 50 : 3 : 1. The product eluents were concentrated to dryness, the resulting material was dissolved in minimal amounts of ethanol/water, and the product was precipitated by the addition of excess solid NH_4PF_6. The orange precipitate was centrifuged, washed twice with water, and dried under high vacuum to afford Δ-[Ru(bpy)(dmb)(phen)](PF$_6$)$_2$ (7.8 mg, 86%). The enantiomeric ratio

(98:2 e.r.) of the product was determined by chiral HPLC analysis (Figure S16) and the absolute metal-centered configuration was assigned by CD spectroscopy (Figure S11). CD (MeCN): λ, nm (Δε, $M^{-1}cm^{-1}$) 294 (-181), 264 (+71).

Synthesis of Δ-[Os(bpy)$_3$](PF$_6$)$_2$ (Δ-6)

In a sealed brown glass vial fitted with a septum, a solution of Δ-**5** (8.1 mg, 0.0090 mmol, 1.0 eq), trifluoroacetic acid (13.5 μL, 0.18 mmol, 20 eq), and 2,2'-bipyridine (43.5 mg, 0.28 mmol, 30 eq) in acetylacetone (0.18 mL) was heated at 150 °C (oil bath temperature) for 5 h under an argon atmosphere. The reaction mixture was cooled to room temperature. The crude material was subjected to silica gel chromatography with acetonitrile and later CH_3CN: H_2O: KNO_3(sat) =60:3:1. The product eluents were concentrated to dryness, the resulting material was dissolved in minimal amounts of ethanol/water, and the product was precipitated by the addition of excess solid NH_4PF_6. The orange precipitate was centrifuged, washed twice with water, and dried under high vacuum to afford Δ-[Os(bpy)$_3$](PF$_6$)$_2$ (4.7 mg, 55%) with 84:1 e.r. The enantiomeric ratio of the product was determined by chiral HPLC analysis (Figure S17). The metal-centered configuration was assigned by comparison with Δ-**5** and by CD spectroscopy (Figure S12).

^{1}H-NMR (400.1 MHz, CH_3CN): δ (ppm) 8.51 (d, J = 8.4 Hz, 6H), 7.89 (dd, J = 8.0, 1.2 Hz, 6H), 7.66 (d, J = 6.0 Hz, 6H), 7.33 (td, J = 5.6, 0.8 Hz, 6H).

^{13}C-NMR (100.6 MHz, CH_3CN): δ (ppm) 158.9, 150.8, 137.1, 128.0, 124.8, 117.3.

IR (film): ν (cm^{-1}) 3356, 3195, 2922, 2851, 1658, 1632, 1462, 1446, 1422, 1180, 1142, 1075, 1026, 887, 838, 762, 728, 659, 558.

HRMS calcd for $C_{15}H_{12}N_3Os$ $[(M-2PF_6)/2]^+$ 330.0839, found: 330.0835.

CD (MeCN): λ, nm (Δε, $M^{-1}cm^{-1}$) 296 (-183), 282 (+70).

5. CD Spectra of Ruthenium and Osmium Complexes

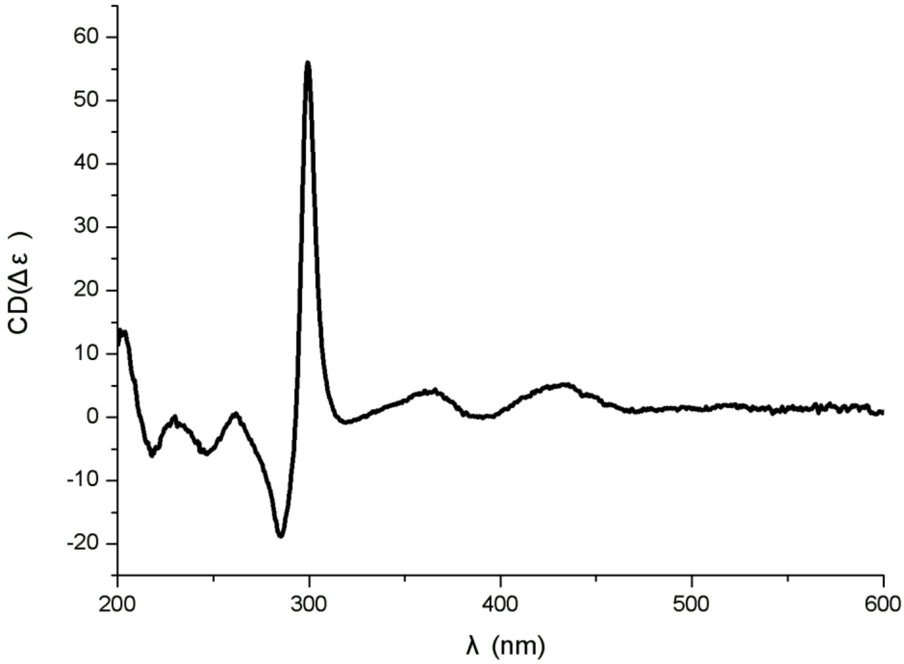


Figure S1. CD spectrum of Λ-**3a** recorded in CH_3CN (0.2 mM).

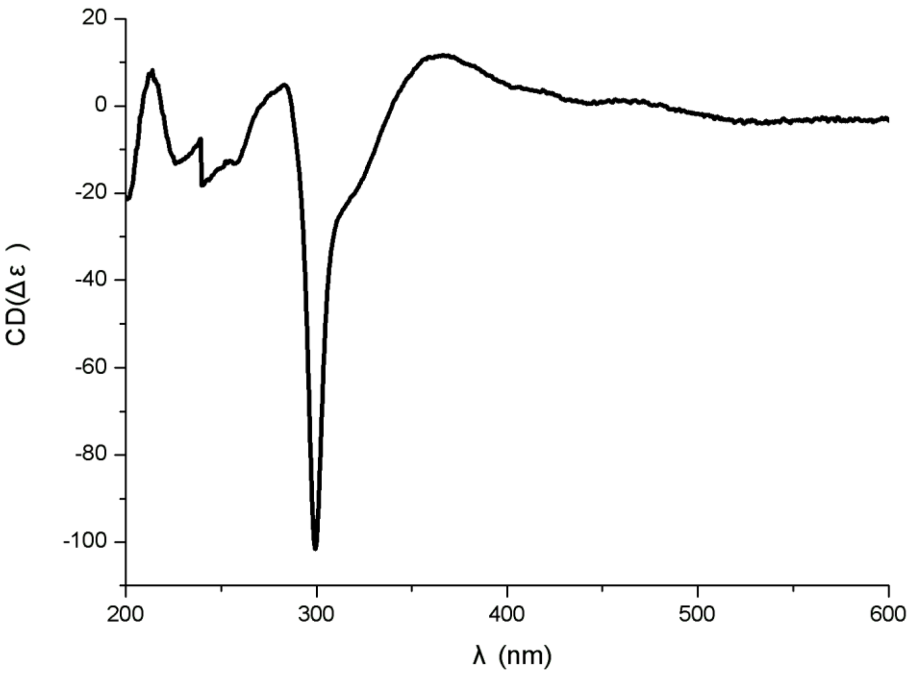


Figure S2. CD spectrum of Δ-**3b** recorded in CH_3CN (0.2 mM).

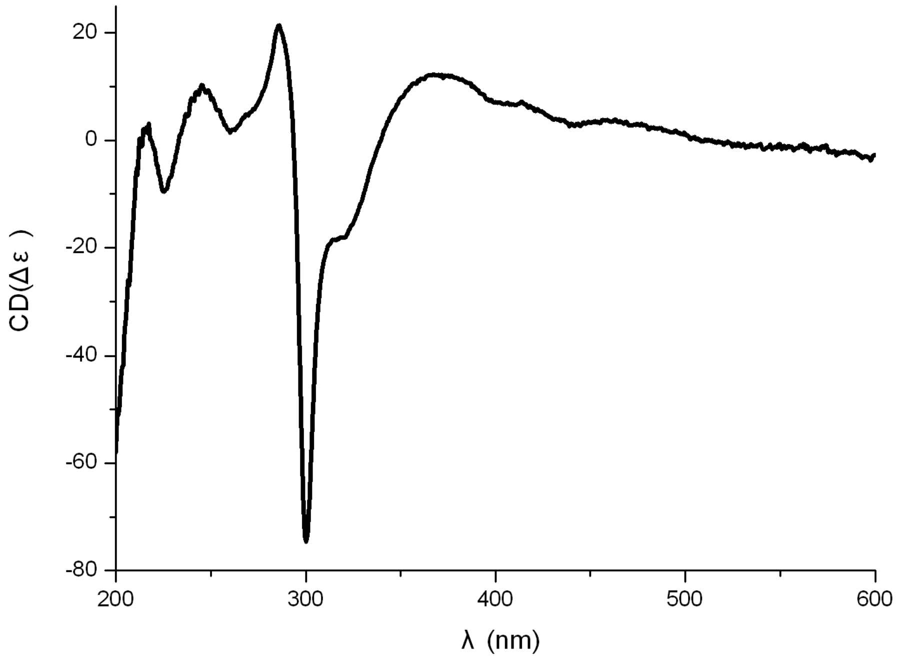


Figure S3. CD spectrum of Δ-**3c** recorded in CH_3CN (0.2 mM).

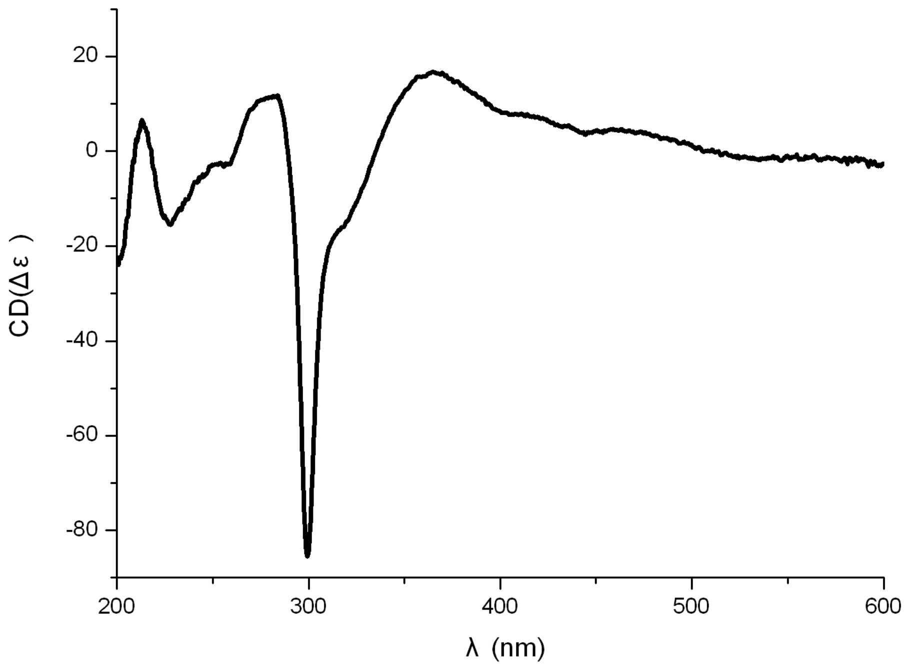


Figure S4. CD spectrum of Δ-**3d** recorded in CH_3CN (0.2 mM).

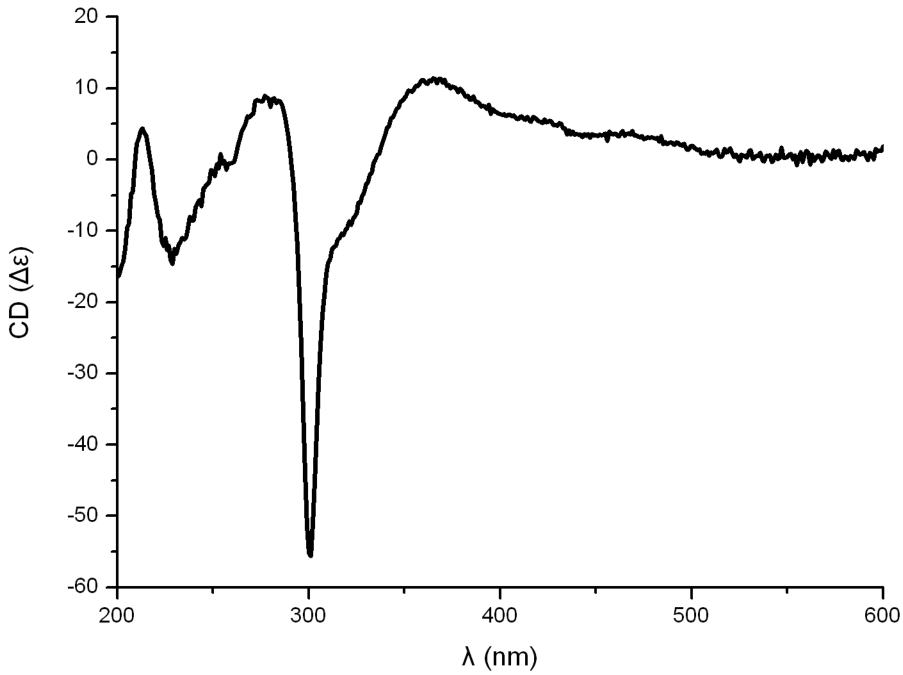


Figure S5. CD spectrum of Δ-**3e** recorded in CH_3CN (0.2 mM).

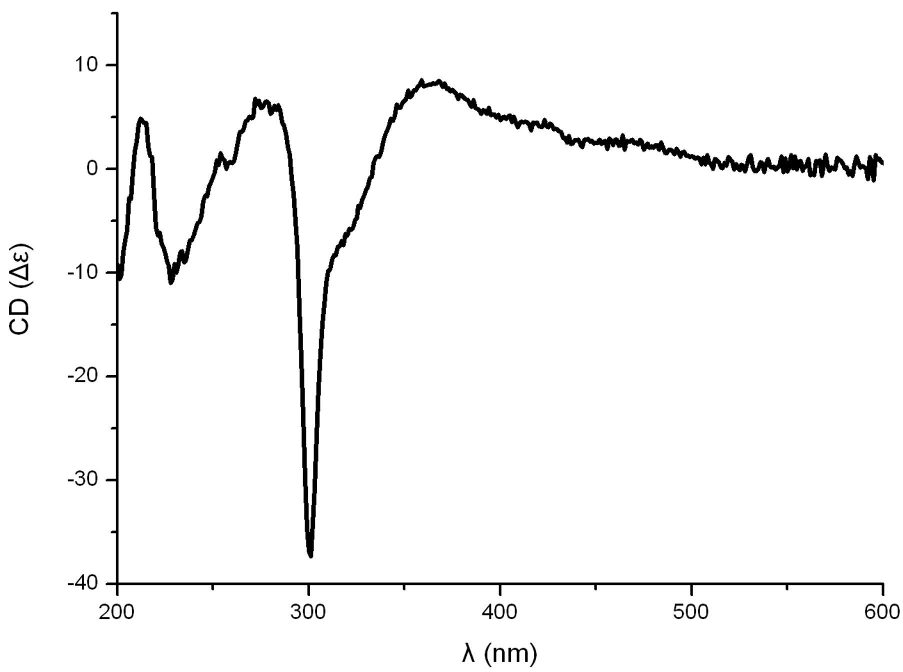


Figure S6. CD spectrum of Δ-**3f** recorded in CH_3CN (0.2 mM).

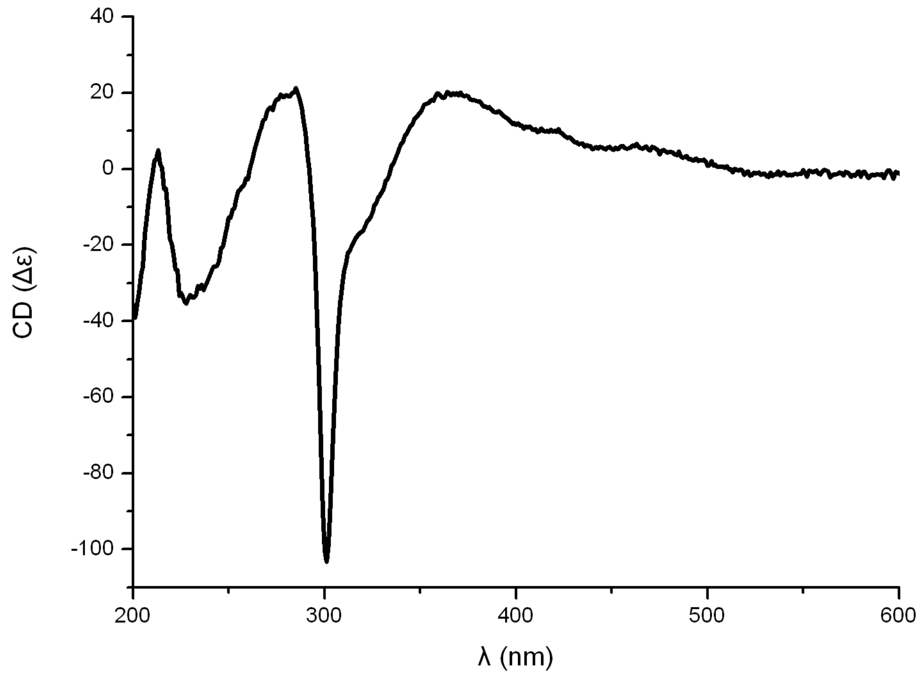


Figure S7. CD spectrum of Δ-**3g** recorded in CH_3CN (0.2 mM).

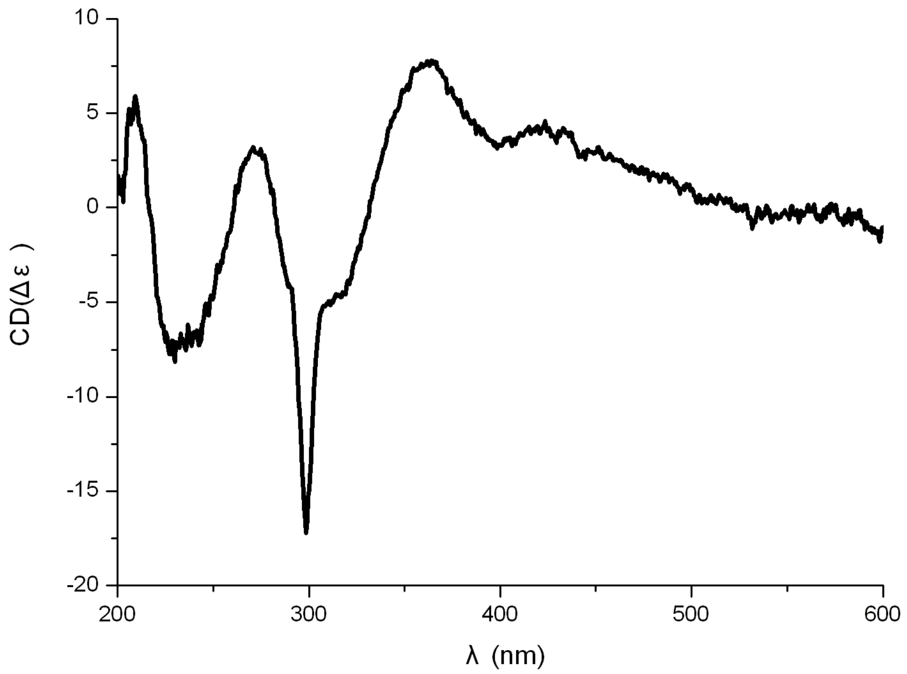


Figure S8. CD spectrum of Δ-**3h** recorded in CH_3CN (0.2 mM).

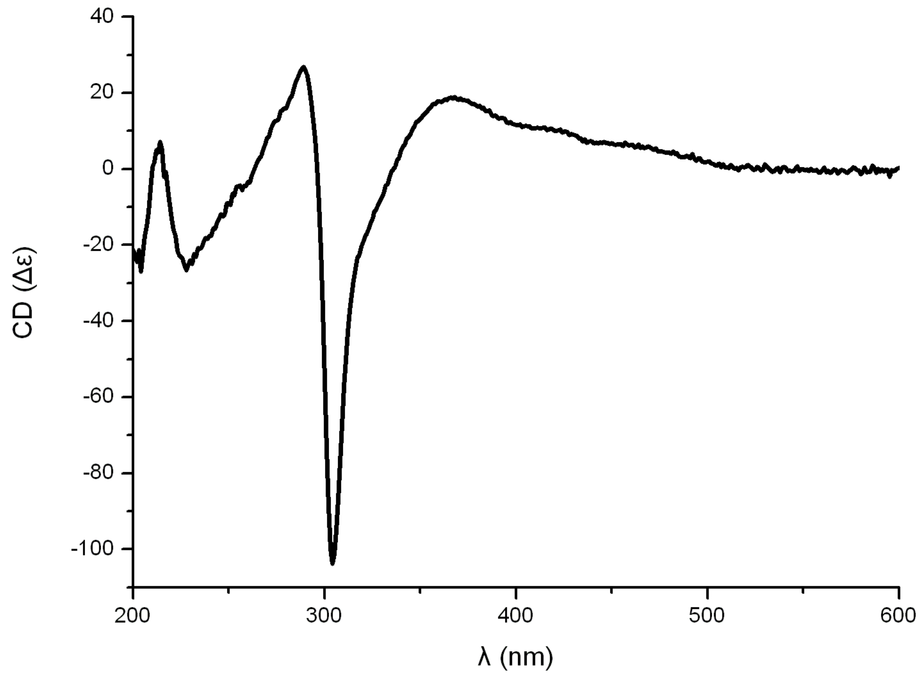


Figure S9. CD spectrum of Δ-[Ru(bpy)(dmp)(**2g**-H)]PF_6 recorded in CH_3CN (0.2 mM).

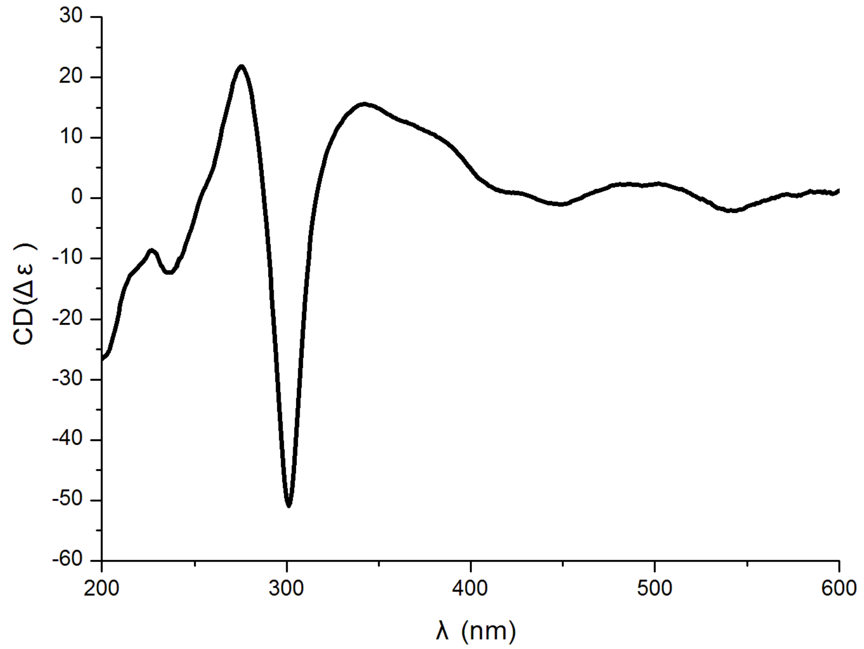


Figure S10. CD spectrum of Δ-**5** recorded in CH_3OH (0.2 mM).

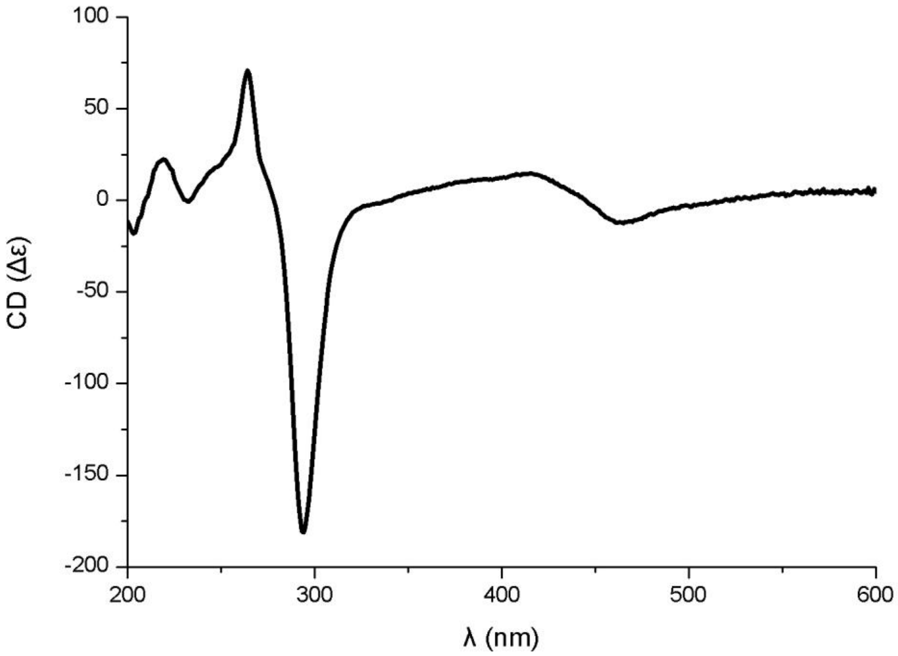


Figure S11. CD spectrum of Δ-[Ru(bpy)(dmb)(phen)]$(PF_6)_2$ recorded in CH_3CN (0.2 mM).

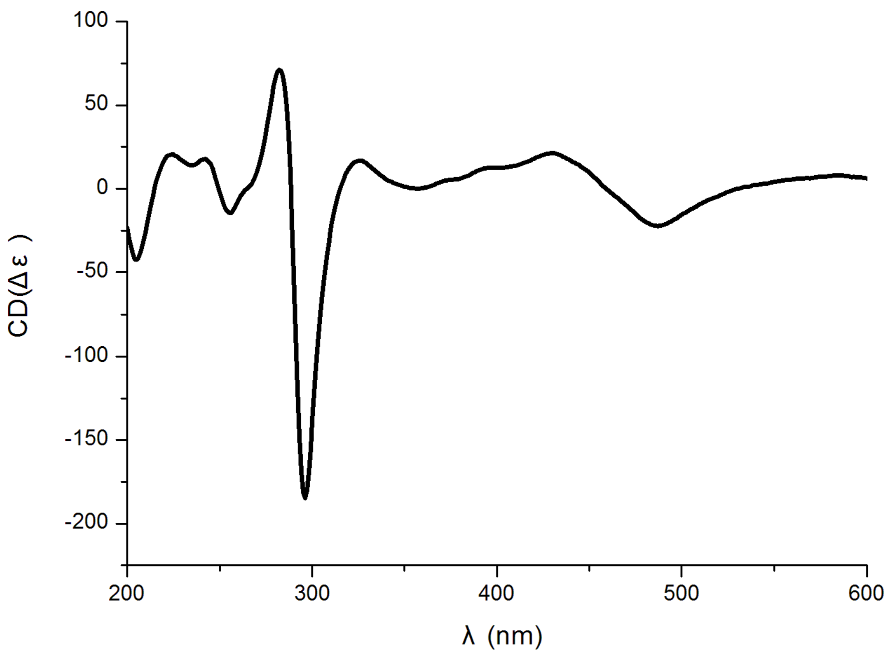


Figure S12. CD spectrum of Δ-**6** recorded in CH_3OH (0.2 mM).

6. Chiral HPLC Chromatography for the Determination of Enantiomeric Ratios

***Δ-[Ru(bpy)$_3$](PF$_6$)$_2$*:** The analysis was performed with a Daicel Chiralpak IA (250 × 4.6 mm) HPLC column on an Agilent 1260 Series HPLC System. The flow rate was 0.75 mL/min, the column temperature was 40 °C, and UV-absorption was measured at 450 nm. Solvent A = 0.1% TFA, solvent B = MeCN, with a linear gradient of 12% to 27% B in 25 min.

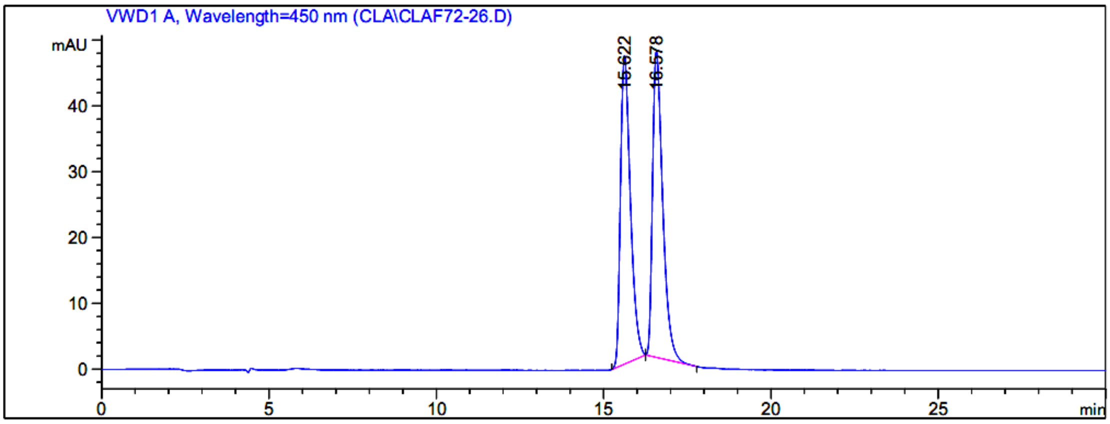


Figure S13. HPLC trace for the racemic reference complex Δ/Λ-[Ru(bpy)$_3$](PF$_6$)$_2$.

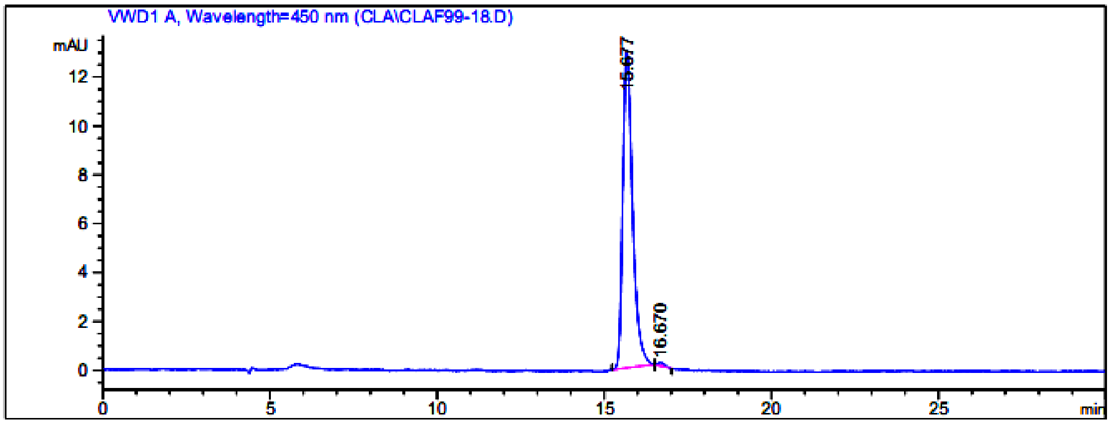


Figure S14. HPLC trace for the complex Δ-[Ru(bpy)$_3$](PF$_6$)$_2$ synthesized from Δ-**3g** (d.r. > 100:1). Integration of peak areas: 100:1 e.r.

***Δ*-[Ru(bpy)(dmb)(phen)](PF_6)$_2$:** The ruthenium complex was analyzed with a Daicel Chiralcel OD-R (250 × 4 mm) HPLC column on an Agilent 1260 Series HPLC System. Flow rate = 0.5 mL/min, the column temperature = 40℃, and UV-absorption measured at 450 nm, solvent A = 0.087% H_3PO_4, solvent B = MeCN, with a linear gradient of 8% to 20% B in 20 min.

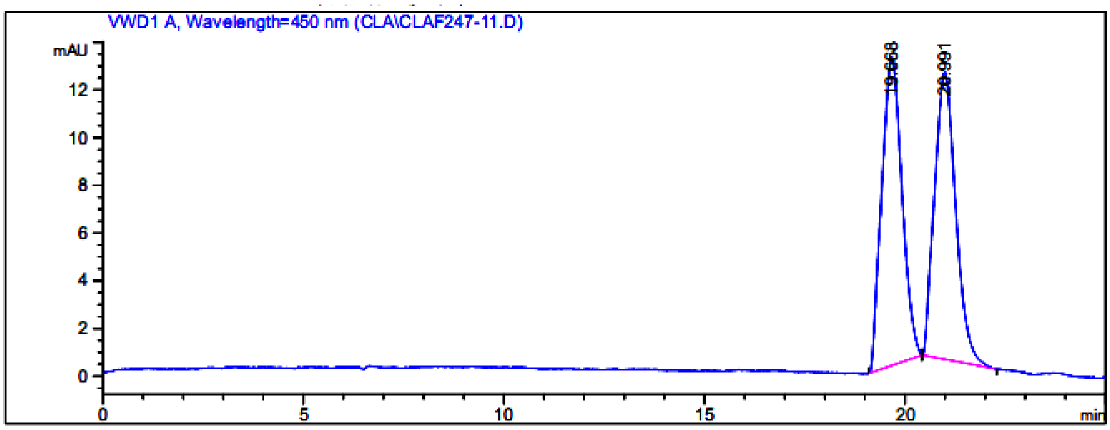


Figure S15. HPLC trace for racemic reference complex Δ/Λ-[Ru(bpy)(dmb)(phen)](PF_6)$_2$.

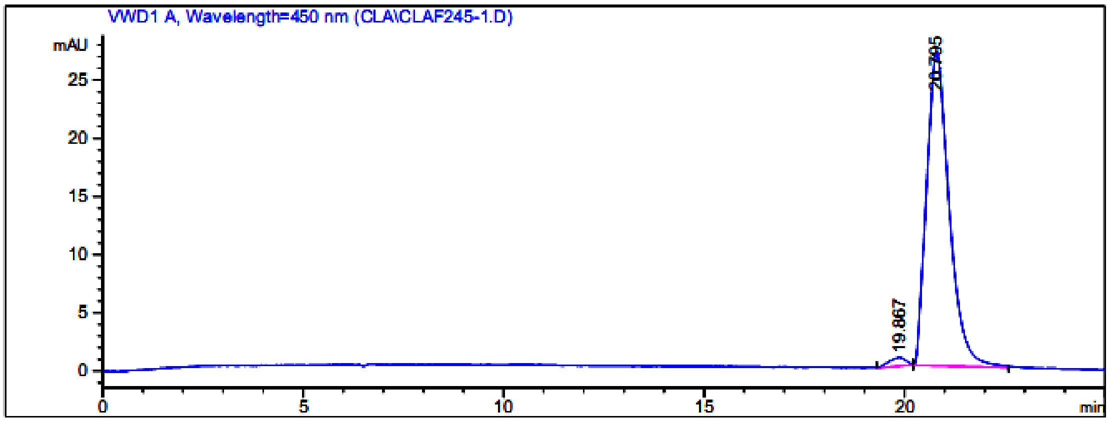


Figure S16. HPLC trace for the complex Δ-[Ru(bpy)(dmb)(phen)](PF_6)$_2$ synthesized from Δ-[Ru(bpy)(dmp)(**2g**-H)]PF_6. Integration of peak areas: 98:2 e.r.

***Δ*-[Os(bpy)$_3$](PF_6)$_2$ (Δ-6):** The analysis was performed with a Daicel Chiralpak IA (250 × 4.6 mm) HPLC column on an Agilent 1260 Series HPLC System. The flow rate was 0.75 mL/min, the column temperature was 40 °C, and UV-absorption was measured at 450 nm. Solvent A = 0.087%

H_3PO_4, solvent B = MeCN, with a linear gradient of 8% to 16% B in 25 min.

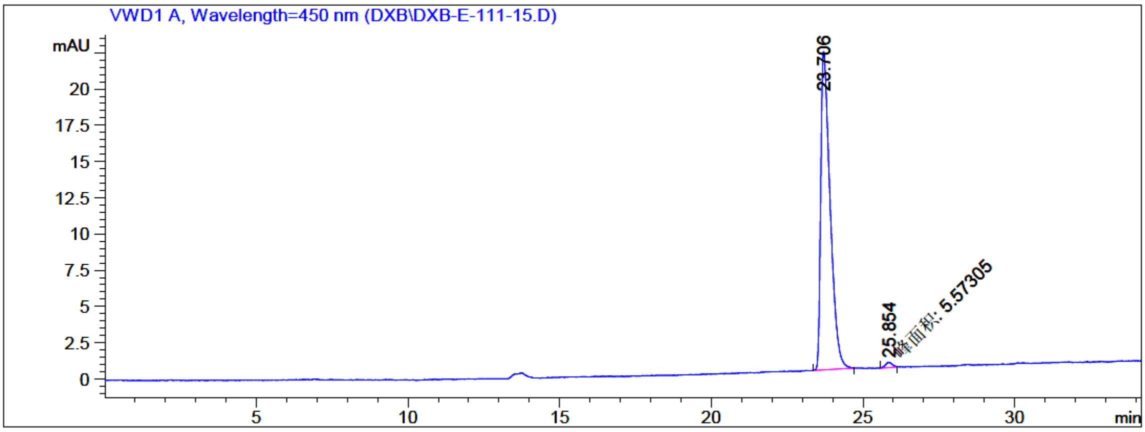


Figure S17. HPLC trace for complex Δ-**6** synthesized from Δ-**5**. Integration of peak areas: 84:1 e.r.

7. Single Crystal X-Ray Diffraction with Ruthenium Complex Δ-3g and Osmium complex Δ-5

Crystals of Δ-**3g** were obtained by slow diffusion from a solution in CH_2Cl_2 layered with Et_2O. Data were collected on an Oxford Xcalibur, Sapphire3, Gemini ultra detector employing graphite-monochromated Mo-K_α radiation (λ = 0.71073 Å) at a temperature of 100 K. The structure was solved by SHELXS-97. Refinement was done by full-matrix least squares based on F^2 data of one twin domain using SHELXL-97. The absolute configuration was determined. The detailed information is listed in the Tables S1-S6.

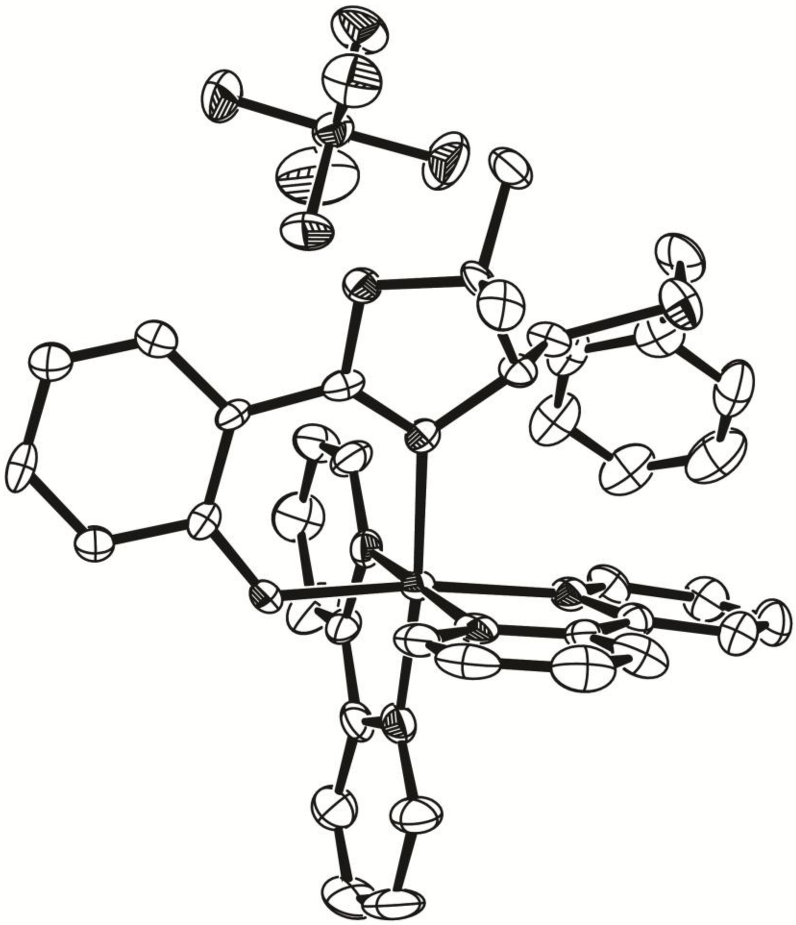


Figure S18. ORTEP drawing of one of the two independent molecules of compound Δ-**3g** with 50% probability thermal ellipsoids. One solvent molecule (methylene chloride) was omitted for clarity.

Table S1. Crystal data and structure refinement for Δ-**3g** (cla1).

Identification code	cla1	
Empirical formula	C78.50 H73 Cl F12 N10 O4 P2 Ru2 S2	
Formula weight	1812.12	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 14.3379(5) Å	α= 90°
	b = 14.9255(5) Å	β= 90°
	c = 37.3985(13) Å	γ = 90°
Volume	8003.3(5) $Å^3$	
Z	4	
Density (calculated)	1.504 Mg/m^3	
Absorption coefficient	0.586 mm^{-1}	
F(000)	3684	
Crystal size	0.30 x 0.17 x 0.12 mm^3	
Theta range for data collection	2.72 to 26.00°.	
Index ranges	-17<=h<=11, -18<=k<=9, -46<=l<=46	
Reflections collected	26584	
Independent reflections	14228 [R(int) = 0.0754]	
Completeness to theta = 26.00°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9330 and 0.8437	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14228 / 41 / 1046	
Goodness-of-fit on F^2	1.001	
Final R indices [I>2sigma(I)]	R1 = 0.0666, wR2 = 0.1047	
R indices (all data)	R1 = 0.0986, wR2 = 0.1155	
Absolute structure parameter	0.05(3)	
Largest diff. peak and hole	0.774 and -0.565 e.$Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x10^3) for Δ-**3g** (cla1). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	6767(1)	3115(1)	7568(1)	18(1)
P(1)	3298(2)	5499(1)	9155(1)	31(1)
Ru(2)	7364(1)	4265(1)	9900(1)	21(1)
P(2)	5555(2)	4201(2)	11626(1)	37(1)
F(11)	3785(4)	6117(4)	8874(2)	87(2)
S(11)	8730(1)	5850(2)	8010(1)	35(1)
O(11)	5763(3)	2976(3)	7185(1)	28(1)
N(11)	6744(4)	4487(3)	7478(1)	20(1)
F(12)	2958(3)	4829(4)	8853(1)	67(2)
O(12)	6231(4)	5769(3)	7242(1)	31(1)
N(12)	7643(4)	2820(3)	7148(1)	20(1)
F(13)	4226(3)	4937(4)	9208(1)	56(2)
N(13)	6767(4)	1760(3)	7593(1)	23(1)
F(14)	2806(3)	4883(3)	9448(1)	53(1)
N(14)	7639(4)	3172(4)	7995(1)	22(1)
F(15)	3613(4)	6149(3)	9475(1)	63(2)
N(15)	5847(4)	3344(4)	7969(2)	23(2)
F(16)	2359(3)	6056(3)	9111(1)	53(1)
F(21)	5712(4)	4766(3)	11273(1)	54(2)
S(21)	4891(2)	6248(1)	10483(1)	39(1)
O(21)	7373(3)	3134(3)	9587(1)	30(1)
N(21)	5954(4)	4076(4)	9992(1)	21(1)
F(22)	4488(3)	4084(3)	11531(1)	57(2)
O(22)	4552(3)	3429(3)	9945(1)	25(1)
N(22)	8717(4)	4419(4)	9752(2)	28(2)
F(23)	5321(4)	5105(3)	11839(1)	52(1)
N(23)	7223(4)	4994(4)	9436(2)	27(2)
F(24)	6626(3)	4325(4)	11727(1)	59(2)
N(24)	7512(4)	5287(4)	10259(2)	25(1)
F(25)	5802(3)	3292(3)	11424(1)	45(1)
N(25)	7540(4)	3575(4)	10365(2)	25(1)
F(26)	5409(4)	3650(3)	11991(1)	60(2)
C(111)	5635(5)	3522(5)	6917(2)	23(2)

C(112)	5209(6)	3157(6)	6603(2)	38(2)
C(113)	5011(7)	3712(7)	6314(2)	49(3)
C(114)	5180(6)	4625(6)	6323(2)	36(2)
C(115)	5596(5)	4981(5)	6621(2)	33(2)
C(116)	5827(5)	4456(5)	6917(2)	20(2)
C(121)	8107(5)	3389(5)	6946(2)	26(2)
C(122)	8481(5)	3160(5)	6616(2)	33(2)
C(123)	8352(6)	2287(5)	6498(2)	31(2)
C(124)	7883(5)	1682(5)	6704(2)	25(2)
C(125)	7549(5)	1952(5)	7035(2)	22(2)
C(131)	6430(6)	1226(5)	7858(2)	33(2)
C(132)	6437(6)	315(5)	7841(2)	35(2)
C(133)	6780(6)	-94(4)	7546(2)	38(2)
C(134)	7127(5)	416(5)	7261(2)	32(2)
C(135)	7115(5)	1342(4)	7298(2)	20(2)
C(141)	8562(5)	2997(5)	7997(2)	27(2)
C(142)	9092(6)	3028(5)	8301(2)	34(2)
C(143)	8688(6)	3253(6)	8618(2)	41(2)
C(144)	7739(6)	3428(5)	8631(2)	35(2)
C(145)	7220(5)	3374(5)	8319(2)	26(2)
C(151)	4922(5)	3392(6)	7930(2)	34(2)
C(152)	4333(6)	3549(6)	8202(2)	40(2)
C(153)	4704(7)	3668(6)	8544(3)	51(3)
C(154)	5632(6)	3632(5)	8590(2)	39(2)
C(155)	6206(5)	3465(5)	8298(2)	20(2)
C(160)	9916(5)	5868(5)	7863(2)	36(2)
C(161)	10460(5)	4997(5)	7929(2)	31(2)
C(162)	10802(6)	4780(6)	8256(2)	34(2)
C(163)	11286(5)	4001(6)	8312(2)	38(2)
C(164)	11442(6)	3428(6)	8040(2)	39(2)
C(165)	11110(6)	3607(6)	7704(2)	43(2)
C(166)	10618(5)	4393(6)	7644(2)	43(2)
C(171)	6277(5)	4876(5)	7222(2)	26(2)
C(172)	6544(6)	6017(5)	7599(2)	32(2)
C(173)	5691(6)	6100(6)	7830(2)	46(2)
C(174)	7047(6)	6911(5)	7561(3)	60(3)
C(175)	7143(5)	5192(4)	7707(2)	19(2)
C(176)	8179(5)	5223(5)	7652(2)	26(2)
C(211)	6653(5)	2719(5)	9456(2)	23(2)

C(212)	6824(5)	2042(4)	9194(2)	26(2)
C(213)	6110(6)	1608(5)	9027(2)	31(2)
C(214)	5178(5)	1787(6)	9112(2)	34(2)
C(215)	5001(5)	2412(5)	9370(2)	30(2)
C(216)	5702(5)	2879(5)	9545(2)	18(2)
C(221)	9461(5)	4090(5)	9930(2)	40(2)
C(222)	10358(6)	4149(6)	9801(3)	52(3)
C(223)	10500(6)	4546(6)	9475(3)	53(3)
C(224)	9761(6)	4897(6)	9293(2)	42(2)
C(225)	8861(6)	4822(5)	9434(2)	31(2)
C(231)	6421(5)	5267(5)	9286(2)	33(2)
C(232)	6377(6)	5723(6)	8971(2)	37(2)
C(233)	7171(7)	5935(7)	8803(2)	52(3)
C(234)	8017(6)	5677(7)	8952(2)	51(3)
C(235)	8040(5)	5181(5)	9261(2)	28(2)
C(241)	7576(6)	6178(4)	10179(2)	29(2)
C(242)	7746(6)	6804(5)	10432(2)	37(2)
C(243)	7849(6)	6570(5)	10780(2)	40(2)
C(244)	7792(5)	5677(5)	10866(2)	35(2)
C(245)	7634(5)	5047(5)	10605(2)	23(2)
C(251)	7495(5)	2680(5)	10396(2)	30(2)
C(252)	7524(5)	2261(5)	10727(2)	36(2)
C(253)	7588(6)	2763(5)	11035(2)	40(2)
C(254)	7638(6)	3684(5)	11001(2)	37(2)
C(255)	7598(5)	4079(5)	10666(2)	23(2)
C(260)	4557(6)	7222(5)	10221(2)	47(2)
C(261)	5357(6)	7634(5)	10013(2)	38(2)
C(262)	5548(6)	7394(5)	9662(2)	36(2)
C(263)	6283(7)	7785(5)	9482(2)	46(2)
C(264)	6841(7)	8416(6)	9644(2)	51(3)
C(265)	6669(8)	8662(6)	9991(3)	67(3)
C(266)	5924(7)	8269(6)	10177(2)	51(3)
C(271)	5456(5)	3491(5)	9833(2)	21(2)
C(272)	4511(5)	3931(5)	10290(2)	24(2)
C(273)	4643(6)	3244(5)	10585(2)	31(2)
C(274)	3548(5)	4342(5)	10307(2)	34(2)
C(275)	5370(5)	4550(4)	10265(2)	21(2)
C(276)	5194(5)	5502(4)	10123(2)	28(2)
C(1S)	8622(7)	8948(8)	8612(4)	33(4)

Cl(1A)	9032(7)	7756(6)	8675(3)	59(3)
Cl(1B)	8702(6)	7993(5)	8391(2)	32(2)
Cl(2A)	7405(10)	8796(11)	8591(4)	48(4)
Cl(2B)	7406(10)	9159(10)	8689(4)	20(4)
Cl(2C)	7539(8)	9420(9)	8763(4)	15(3)

Table S3. Bond lengths [Å] and angles [°] for Δ-**3g** (cla1).

Ru(1)-N(13)	2.024(5)
Ru(1)-N(15)	2.025(6)
Ru(1)-N(14)	2.030(6)
Ru(1)-O(11)	2.043(5)
Ru(1)-N(12)	2.058(5)
Ru(1)-N(11)	2.075(5)
P(1)-F(11)	1.563(6)
P(1)-F(13)	1.586(5)
P(1)-F(12)	1.587(5)
P(1)-F(16)	1.591(5)
P(1)-F(14)	1.597(5)
P(1)-F(15)	1.606(5)
Ru(2)-N(22)	2.029(6)
Ru(2)-N(25)	2.038(6)
Ru(2)-N(24)	2.045(5)
Ru(2)-O(21)	2.053(5)
Ru(2)-N(23)	2.056(6)
Ru(2)-N(21)	2.071(6)
P(2)-F(22)	1.580(5)
P(2)-F(21)	1.585(5)
P(2)-F(24)	1.592(5)
P(2)-F(25)	1.593(5)
P(2)-F(23)	1.603(5)
P(2)-F(26)	1.605(5)
S(11)-C(160)	1.787(8)
S(11)-C(176)	1.813(7)
O(11)-C(111)	1.303(8)
N(11)-C(171)	1.306(8)
N(11)-C(175)	1.471(8)
O(12)-C(171)	1.338(8)
O(12)-C(172)	1.457(8)
N(12)-C(121)	1.317(8)
N(12)-C(125)	1.369(8)
N(13)-C(135)	1.360(8)
N(13)-C(131)	1.360(9)
N(14)-C(141)	1.349(9)
N(14)-C(145)	1.384(8)

N(15)-C(151)	1.336(9)
N(15)-C(155)	1.348(8)
S(21)-C(276)	1.800(7)
S(21)-C(260)	1.818(8)
O(21)-C(211)	1.300(8)
N(21)-C(271)	1.275(8)
N(21)-C(275)	1.497(8)
O(22)-C(271)	1.366(8)
O(22)-C(272)	1.492(8)
N(22)-C(221)	1.349(9)
N(22)-C(225)	1.350(9)
N(23)-C(231)	1.344(9)
N(23)-C(235)	1.371(9)
N(24)-C(245)	1.353(8)
N(24)-C(241)	1.365(8)
N(25)-C(251)	1.343(8)
N(25)-C(255)	1.356(8)
C(111)-C(116)	1.421(9)
C(111)-C(112)	1.431(10)
C(112)-C(113)	1.389(11)
C(112)-H(11A)	0.9500
C(113)-C(114)	1.384(11)
C(113)-H(11B)	0.9500
C(114)-C(115)	1.369(10)
C(114)-H(11C)	0.9500
C(115)-C(116)	1.397(9)
C(115)-H(11D)	0.9500
C(116)-C(171)	1.453(9)
C(121)-C(122)	1.389(9)
C(121)-H(12A)	0.9500
C(122)-C(123)	1.388(10)
C(122)-H(12B)	0.9500
C(123)-C(124)	1.363(9)
C(123)-H(12C)	0.9500
C(124)-C(125)	1.389(9)
C(124)-H(12D)	0.9500
C(125)-C(135)	1.477(9)
C(131)-C(132)	1.361(10)
C(131)-H(13A)	0.9500

C(132)-C(133)	1.353(10)
C(132)-H(13B)	0.9500
C(133)-C(134)	1.400(10)
C(133)-H(13C)	0.9500
C(134)-C(135)	1.390(9)
C(134)-H(13D)	0.9500
C(141)-C(142)	1.369(10)
C(141)-H(14A)	0.9500
C(142)-C(143)	1.361(10)
C(142)-H(14B)	0.9500
C(143)-C(144)	1.386(11)
C(143)-H(14C)	0.9500
C(144)-C(145)	1.387(10)
C(144)-H(14D)	0.9500
C(145)-C(155)	1.462(10)
C(151)-C(152)	1.344(10)
C(151)-H(15A)	0.9500
C(152)-C(153)	1.397(12)
C(152)-H(15B)	0.9500
C(153)-C(154)	1.342(12)
C(153)-H(15C)	0.9500
C(154)-C(155)	1.391(10)
C(154)-H(15D)	0.9500
C(160)-C(161)	1.536(10)
C(160)-H(16A)	0.9900
C(160)-H(16B)	0.9900
C(161)-C(162)	1.355(10)
C(161)-C(166)	1.416(11)
C(162)-C(163)	1.370(11)
C(162)-H(16C)	0.9500
C(163)-C(164)	1.346(11)
C(163)-H(16D)	0.9500
C(164)-C(165)	1.370(10)
C(164)-H(16E)	0.9500
C(165)-C(166)	1.389(11)
C(165)-H(16F)	0.9500
C(166)-H(16G)	0.9500
C(172)-C(173)	1.502(11)
C(172)-C(174)	1.525(10)

C(172)-C(175)	1.553(9)
C(173)-H(17A)	0.9800
C(173)-H(17B)	0.9800
C(173)-H(17C)	0.9800
C(174)-H(17D)	0.9800
C(174)-H(17E)	0.9800
C(174)-H(17F)	0.9800
C(175)-C(176)	1.501(9)
C(175)-H(17G)	1.0000
C(176)-H(17H)	0.9900
C(176)-H(17I)	0.9900
C(211)-C(216)	1.422(10)
C(211)-C(212)	1.430(9)
C(212)-C(213)	1.362(9)
C(212)-H(21A)	0.9500
C(213)-C(214)	1.399(10)
C(213)-H(21B)	0.9500
C(214)-C(215)	1.366(10)
C(214)-H(21C)	0.9500
C(215)-C(216)	1.388(9)
C(215)-H(21D)	0.9500
C(216)-C(271)	1.457(9)
C(221)-C(222)	1.376(11)
C(221)-H(22A)	0.9500
C(222)-C(223)	1.371(12)
C(222)-H(22B)	0.9500
C(223)-C(224)	1.364(12)
C(223)-H(22C)	0.9500
C(224)-C(225)	1.398(10)
C(224)-H(22D)	0.9500
C(225)-C(235)	1.446(11)
C(231)-C(232)	1.361(10)
C(231)-H(23A)	0.9500
C(232)-C(233)	1.340(11)
C(232)-H(23B)	0.9500
C(233)-C(234)	1.390(11)
C(233)-H(23C)	0.9500
C(234)-C(235)	1.373(10)
C(234)-H(23D)	0.9500

C(241)-C(242)	1.353(9)
C(241)-H(24A)	0.9500
C(242)-C(243)	1.355(10)
C(242)-H(24B)	0.9500
C(243)-C(244)	1.372(10)
C(243)-H(24C)	0.9500
C(244)-C(245)	1.375(9)
C(244)-H(24D)	0.9500
C(245)-C(255)	1.463(9)
C(251)-C(252)	1.389(10)
C(251)-H(25A)	0.9500
C(252)-C(253)	1.375(10)
C(252)-H(25B)	0.9500
C(253)-C(254)	1.382(10)
C(253)-H(25C)	0.9500
C(254)-C(255)	1.386(9)
C(254)-H(25D)	0.9500
C(260)-C(261)	1.516(12)
C(260)-H(26A)	0.9900
C(260)-H(26B)	0.9900
C(261)-C(262)	1.390(11)
C(261)-C(266)	1.391(11)
C(262)-C(263)	1.379(11)
C(262)-H(26C)	0.9500
C(263)-C(264)	1.377(11)
C(263)-H(26D)	0.9500
C(264)-C(265)	1.371(12)
C(264)-H(26E)	0.9500
C(265)-C(266)	1.404(13)
C(265)-H(26F)	0.9500
C(266)-H(26G)	0.9500
C(272)-C(274)	1.513(9)
C(272)-C(273)	1.519(9)
C(272)-C(275)	1.543(10)
C(273)-H(27A)	0.9800
C(273)-H(27B)	0.9800
C(273)-H(27C)	0.9800
C(274)-H(27D)	0.9800
C(274)-H(27E)	0.9800

C(274)-H(27F)	0.9800
C(275)-C(276)	1.537(9)
C(275)-H(27G)	1.0000
C(276)-H(27H)	0.9900
C(276)-H(27I)	0.9900
C(1S)-Cl(1B)	1.651(12)
C(1S)-Cl(2A)	1.761(15)
C(1S)-Cl(2B)	1.795(16)
C(1S)-Cl(2C)	1.796(14)
C(1S)-Cl(1A)	1.888(13)
C(1S)-H(1SA)	0.9900
C(1S)-H(1SB)	0.9900
Cl(1A)-Cl(1B)	1.216(12)
Cl(2A)-Cl(2B)	0.656(17)
Cl(2A)-Cl(2C)	1.15(2)
Cl(2B)-Cl(2C)	0.514(15)

N(13)-Ru(1)-N(15)	97.8(2)
N(13)-Ru(1)-N(14)	90.4(2)
N(15)-Ru(1)-N(14)	79.2(2)
N(13)-Ru(1)-O(11)	86.0(2)
N(15)-Ru(1)-O(11)	94.5(2)
N(14)-Ru(1)-O(11)	172.2(2)
N(13)-Ru(1)-N(12)	79.7(2)
N(15)-Ru(1)-N(12)	176.3(2)
N(14)-Ru(1)-N(12)	103.5(2)
O(11)-Ru(1)-N(12)	82.7(2)
N(13)-Ru(1)-N(11)	173.2(2)
N(15)-Ru(1)-N(11)	86.7(2)
N(14)-Ru(1)-N(11)	95.5(2)
O(11)-Ru(1)-N(11)	88.6(2)
N(12)-Ru(1)-N(11)	95.6(2)
F(11)-P(1)-F(13)	91.2(3)
F(11)-P(1)-F(12)	91.7(3)
F(13)-P(1)-F(12)	90.8(3)
F(11)-P(1)-F(16)	90.0(3)
F(13)-P(1)-F(16)	178.7(3)
F(12)-P(1)-F(16)	89.7(3)
F(11)-P(1)-F(14)	178.8(3)

F(13)-P(1)-F(14)	88.9(3)
F(12)-P(1)-F(14)	89.4(3)
F(16)-P(1)-F(14)	89.9(3)
F(11)-P(1)-F(15)	91.1(3)
F(13)-P(1)-F(15)	89.5(3)
F(12)-P(1)-F(15)	177.1(3)
F(16)-P(1)-F(15)	89.9(3)
F(14)-P(1)-F(15)	87.7(3)
N(22)-Ru(2)-N(25)	99.8(2)
N(22)-Ru(2)-N(24)	89.7(2)
N(25)-Ru(2)-N(24)	78.6(2)
N(22)-Ru(2)-O(21)	86.2(2)
N(25)-Ru(2)-O(21)	94.0(2)
N(24)-Ru(2)-O(21)	170.8(2)
N(22)-Ru(2)-N(23)	78.8(2)
N(25)-Ru(2)-N(23)	177.9(3)
N(24)-Ru(2)-N(23)	99.7(2)
O(21)-Ru(2)-N(23)	87.5(2)
N(22)-Ru(2)-N(21)	173.7(2)
N(25)-Ru(2)-N(21)	84.9(2)
N(24)-Ru(2)-N(21)	95.4(2)
O(21)-Ru(2)-N(21)	89.4(2)
N(23)-Ru(2)-N(21)	96.7(2)
F(22)-P(2)-F(21)	90.5(3)
F(22)-P(2)-F(24)	179.2(3)
F(21)-P(2)-F(24)	89.9(3)
F(22)-P(2)-F(25)	90.8(3)
F(21)-P(2)-F(25)	91.4(3)
F(24)-P(2)-F(25)	89.8(3)
F(22)-P(2)-F(23)	90.1(3)
F(21)-P(2)-F(23)	89.8(3)
F(24)-P(2)-F(23)	89.2(3)
F(25)-P(2)-F(23)	178.4(3)
F(22)-P(2)-F(26)	90.5(3)
F(21)-P(2)-F(26)	178.5(3)
F(24)-P(2)-F(26)	89.1(3)
F(25)-P(2)-F(26)	89.8(3)
F(23)-P(2)-F(26)	89.0(3)
C(160)-S(11)-C(176)	101.3(4)

C(111)-O(11)-Ru(1)	125.1(5)
C(171)-N(11)-C(175)	107.8(6)
C(171)-N(11)-Ru(1)	124.5(5)
C(175)-N(11)-Ru(1)	127.4(4)
C(171)-O(12)-C(172)	106.7(5)
C(121)-N(12)-C(125)	118.8(6)
C(121)-N(12)-Ru(1)	127.4(4)
C(125)-N(12)-Ru(1)	112.2(4)
C(135)-N(13)-C(131)	116.8(6)
C(135)-N(13)-Ru(1)	114.9(4)
C(131)-N(13)-Ru(1)	128.2(5)
C(141)-N(14)-C(145)	117.7(6)
C(141)-N(14)-Ru(1)	126.8(5)
C(145)-N(14)-Ru(1)	115.5(5)
C(151)-N(15)-C(155)	118.2(7)
C(151)-N(15)-Ru(1)	125.1(5)
C(155)-N(15)-Ru(1)	116.7(5)
C(276)-S(21)-C(260)	98.9(4)
C(211)-O(21)-Ru(2)	127.0(4)
C(271)-N(21)-C(275)	109.2(5)
C(271)-N(21)-Ru(2)	124.2(5)
C(275)-N(21)-Ru(2)	126.5(4)
C(271)-O(22)-C(272)	105.5(5)
C(221)-N(22)-C(225)	118.3(7)
C(221)-N(22)-Ru(2)	125.5(5)
C(225)-N(22)-Ru(2)	115.9(5)
C(231)-N(23)-C(235)	118.0(6)
C(231)-N(23)-Ru(2)	126.7(5)
C(235)-N(23)-Ru(2)	115.3(5)
C(245)-N(24)-C(241)	117.3(6)
C(245)-N(24)-Ru(2)	116.3(4)
C(241)-N(24)-Ru(2)	126.1(5)
C(251)-N(25)-C(255)	118.9(6)
C(251)-N(25)-Ru(2)	124.7(5)
C(255)-N(25)-Ru(2)	115.9(4)
O(11)-C(111)-C(116)	125.8(6)
O(11)-C(111)-C(112)	116.9(7)
C(116)-C(111)-C(112)	117.1(6)
C(113)-C(112)-C(111)	119.8(8)

C(113)-C(112)-H(11A)	120.1
C(111)-C(112)-H(11A)	120.1
C(114)-C(113)-C(112)	122.2(8)
C(114)-C(113)-H(11B)	118.9
C(112)-C(113)-H(11B)	118.9
C(115)-C(114)-C(113)	118.5(7)
C(115)-C(114)-H(11C)	120.8
C(113)-C(114)-H(11C)	120.8
C(114)-C(115)-C(116)	122.1(7)
C(114)-C(115)-H(11D)	119.0
C(116)-C(115)-H(11D)	119.0
C(115)-C(116)-C(111)	120.2(6)
C(115)-C(116)-C(171)	119.1(7)
C(111)-C(116)-C(171)	120.6(6)
N(12)-C(121)-C(122)	123.1(7)
N(12)-C(121)-H(12A)	118.4
C(122)-C(121)-H(12A)	118.4
C(123)-C(122)-C(121)	117.5(7)
C(123)-C(122)-H(12B)	121.3
C(121)-C(122)-H(12B)	121.3
C(124)-C(123)-C(122)	120.6(6)
C(124)-C(123)-H(12C)	119.7
C(122)-C(123)-H(12C)	119.7
C(123)-C(124)-C(125)	118.8(6)
C(123)-C(124)-H(12D)	120.6
C(125)-C(124)-H(12D)	120.6
N(12)-C(125)-C(124)	121.1(6)
N(12)-C(125)-C(135)	114.8(5)
C(124)-C(125)-C(135)	124.1(6)
N(13)-C(131)-C(132)	123.3(7)
N(13)-C(131)-H(13A)	118.4
C(132)-C(131)-H(13A)	118.4
C(133)-C(132)-C(131)	119.4(7)
C(133)-C(132)-H(13B)	120.3
C(131)-C(132)-H(13B)	120.3
C(132)-C(133)-C(134)	120.2(6)
C(132)-C(133)-H(13C)	119.9
C(134)-C(133)-H(13C)	119.9
C(135)-C(134)-C(133)	117.4(7)

C(135)-C(134)-H(13D)	121.3
C(133)-C(134)-H(13D)	121.3
N(13)-C(135)-C(134)	122.8(6)
N(13)-C(135)-C(125)	114.3(6)
C(134)-C(135)-C(125)	122.8(6)
N(14)-C(141)-C(142)	122.7(7)
N(14)-C(141)-H(14A)	118.6
C(142)-C(141)-H(14A)	118.6
C(143)-C(142)-C(141)	119.7(7)
C(143)-C(142)-H(14B)	120.1
C(141)-C(142)-H(14B)	120.1
C(142)-C(143)-C(144)	119.7(8)
C(142)-C(143)-H(14C)	120.2
C(144)-C(143)-H(14C)	120.2
C(143)-C(144)-C(145)	119.1(8)
C(143)-C(144)-H(14D)	120.5
C(145)-C(144)-H(14D)	120.5
N(14)-C(145)-C(144)	121.1(7)
N(14)-C(145)-C(155)	113.9(6)
C(144)-C(145)-C(155)	124.9(7)
N(15)-C(151)-C(152)	123.4(8)
N(15)-C(151)-H(15A)	118.3
C(152)-C(151)-H(15A)	118.3
C(151)-C(152)-C(153)	118.5(8)
C(151)-C(152)-H(15B)	120.7
C(153)-C(152)-H(15B)	120.7
C(154)-C(153)-C(152)	119.3(8)
C(154)-C(153)-H(15C)	120.4
C(152)-C(153)-H(15C)	120.4
C(153)-C(154)-C(155)	119.6(8)
C(153)-C(154)-H(15D)	120.2
C(155)-C(154)-H(15D)	120.2
N(15)-C(155)-C(154)	121.0(7)
N(15)-C(155)-C(145)	114.6(6)
C(154)-C(155)-C(145)	124.4(7)
C(161)-C(160)-S(11)	114.9(5)
C(161)-C(160)-H(16A)	108.5
S(11)-C(160)-H(16A)	108.5
C(161)-C(160)-H(16B)	108.5

S(11)-C(160)-H(16B)	108.5
H(16A)-C(160)-H(16B)	107.5
C(162)-C(161)-C(166)	118.0(8)
C(162)-C(161)-C(160)	122.1(8)
C(166)-C(161)-C(160)	119.8(7)
C(161)-C(162)-C(163)	121.6(8)
C(161)-C(162)-H(16C)	119.2
C(163)-C(162)-H(16C)	119.2
C(164)-C(163)-C(162)	120.5(8)
C(164)-C(163)-H(16D)	119.7
C(162)-C(163)-H(16D)	119.7
C(163)-C(164)-C(165)	120.7(8)
C(163)-C(164)-H(16E)	119.7
C(165)-C(164)-H(16E)	119.7
C(164)-C(165)-C(166)	119.4(8)
C(164)-C(165)-H(16F)	120.3
C(166)-C(165)-H(16F)	120.3
C(165)-C(166)-C(161)	119.7(8)
C(165)-C(166)-H(16G)	120.2
C(161)-C(166)-H(16G)	120.2
N(11)-C(171)-O(12)	115.4(7)
N(11)-C(171)-C(116)	127.8(7)
O(12)-C(171)-C(116)	116.8(6)
O(12)-C(172)-C(173)	107.3(6)
O(12)-C(172)-C(174)	106.4(6)
C(173)-C(172)-C(174)	111.5(7)
O(12)-C(172)-C(175)	101.9(5)
C(173)-C(172)-C(175)	111.5(6)
C(174)-C(172)-C(175)	117.1(6)
C(172)-C(173)-H(17A)	109.5
C(172)-C(173)-H(17B)	109.5
H(17A)-C(173)-H(17B)	109.5
C(172)-C(173)-H(17C)	109.5
H(17A)-C(173)-H(17C)	109.5
H(17B)-C(173)-H(17C)	109.5
C(172)-C(174)-H(17D)	109.5
C(172)-C(174)-H(17E)	109.5
H(17D)-C(174)-H(17E)	109.5
C(172)-C(174)-H(17F)	109.5

H(17D)-C(174)-H(17F)	109.5
H(17E)-C(174)-H(17F)	109.5
N(11)-C(175)-C(176)	109.1(6)
N(11)-C(175)-C(172)	101.7(5)
C(176)-C(175)-C(172)	119.3(6)
N(11)-C(175)-H(17G)	108.8
C(176)-C(175)-H(17G)	108.8
C(172)-C(175)-H(17G)	108.8
C(175)-C(176)-S(11)	110.3(5)
C(175)-C(176)-H(17H)	109.6
S(11)-C(176)-H(17H)	109.6
C(175)-C(176)-H(17I)	109.6
S(11)-C(176)-H(17I)	109.6
H(17H)-C(176)-H(17I)	108.1
O(21)-C(211)-C(216)	126.3(6)
O(21)-C(211)-C(212)	117.3(7)
C(216)-C(211)-C(212)	116.3(7)
C(213)-C(212)-C(211)	121.4(7)
C(213)-C(212)-H(21A)	119.3
C(211)-C(212)-H(21A)	119.3
C(212)-C(213)-C(214)	121.5(7)
C(212)-C(213)-H(21B)	119.2
C(214)-C(213)-H(21B)	119.2
C(215)-C(214)-C(213)	117.9(7)
C(215)-C(214)-H(21C)	121.0
C(213)-C(214)-H(21C)	121.1
C(214)-C(215)-C(216)	122.8(7)
C(214)-C(215)-H(21D)	118.6
C(216)-C(215)-H(21D)	118.6
C(215)-C(216)-C(211)	119.9(6)
C(215)-C(216)-C(271)	119.3(6)
C(211)-C(216)-C(271)	120.7(6)
N(22)-C(221)-C(222)	122.9(9)
N(22)-C(221)-H(22A)	118.5
C(222)-C(221)-H(22A)	118.5
C(223)-C(222)-C(221)	118.6(9)
C(223)-C(222)-H(22B)	120.7
C(221)-C(222)-H(22B)	120.7
C(224)-C(223)-C(222)	119.6(8)

C(224)-C(223)-H(22C)	120.2
C(222)-C(223)-H(22C)	120.2
C(223)-C(224)-C(225)	119.9(8)
C(223)-C(224)-H(22D)	120.0
C(225)-C(224)-H(22D)	120.0
N(22)-C(225)-C(224)	120.6(8)
N(22)-C(225)-C(235)	115.8(7)
C(224)-C(225)-C(235)	123.6(7)
N(23)-C(231)-C(232)	123.6(8)
N(23)-C(231)-H(23A)	118.2
C(232)-C(231)-H(23A)	118.2
C(233)-C(232)-C(231)	119.0(8)
C(233)-C(232)-H(23B)	120.5
C(231)-C(232)-H(23B)	120.5
C(232)-C(233)-C(234)	119.2(7)
C(232)-C(233)-H(23C)	120.4
C(234)-C(233)-H(23C)	120.4
C(235)-C(234)-C(233)	120.6(8)
C(235)-C(234)-H(23D)	119.7
C(233)-C(234)-H(23D)	119.7
N(23)-C(235)-C(234)	119.5(7)
N(23)-C(235)-C(225)	114.0(6)
C(234)-C(235)-C(225)	126.5(7)
C(242)-C(241)-N(24)	122.1(7)
C(242)-C(241)-H(24A)	118.9
N(24)-C(241)-H(24A)	118.9
C(241)-C(242)-C(243)	120.8(7)
C(241)-C(242)-H(24B)	119.6
C(243)-C(242)-H(24B)	119.6
C(242)-C(243)-C(244)	117.9(7)
C(242)-C(243)-H(24C)	121.1
C(244)-C(243)-H(24C)	121.0
C(243)-C(244)-C(245)	120.6(7)
C(243)-C(244)-H(24D)	119.7
C(245)-C(244)-H(24D)	119.7
N(24)-C(245)-C(244)	121.2(6)
N(24)-C(245)-C(255)	114.0(6)
C(244)-C(245)-C(255)	124.8(6)
N(25)-C(251)-C(252)	121.5(7)

N(25)-C(251)-H(25A)	119.2
C(252)-C(251)-H(25A)	119.2
C(253)-C(252)-C(251)	120.2(7)
C(253)-C(252)-H(25B)	119.9
C(251)-C(252)-H(25B)	119.9
C(252)-C(253)-C(254)	117.9(7)
C(252)-C(253)-H(25C)	121.0
C(254)-C(253)-H(25C)	121.0
C(253)-C(254)-C(255)	120.3(8)
C(253)-C(254)-H(25D)	119.9
C(255)-C(254)-H(25D)	119.9
N(25)-C(255)-C(254)	121.1(7)
N(25)-C(255)-C(245)	114.8(6)
C(254)-C(255)-C(245)	124.0(6)
C(261)-C(260)-S(21)	113.7(6)
C(261)-C(260)-H(26A)	108.8
S(21)-C(260)-H(26A)	108.8
C(261)-C(260)-H(26B)	108.8
S(21)-C(260)-H(26B)	108.8
H(26A)-C(260)-H(26B)	107.7
C(262)-C(261)-C(266)	118.6(8)
C(262)-C(261)-C(260)	121.9(8)
C(266)-C(261)-C(260)	119.5(8)
C(263)-C(262)-C(261)	120.1(8)
C(263)-C(262)-H(26C)	120.0
C(261)-C(262)-H(26C)	120.0
C(264)-C(263)-C(262)	121.4(9)
C(264)-C(263)-H(26D)	119.3
C(262)-C(263)-H(26D)	119.3
C(265)-C(264)-C(263)	119.6(9)
C(265)-C(264)-H(26E)	120.2
C(263)-C(264)-H(26E)	120.2
C(264)-C(265)-C(266)	119.7(9)
C(264)-C(265)-H(26F)	120.2
C(266)-C(265)-H(26F)	120.2
C(261)-C(266)-C(265)	120.7(9)
C(261)-C(266)-H(26G)	119.7
C(265)-C(266)-H(26G)	119.7
N(21)-C(271)-O(22)	115.8(6)

N(21)-C(271)-C(216)	129.7(6)
O(22)-C(271)-C(216)	114.5(6)
O(22)-C(272)-C(274)	106.0(6)
O(22)-C(272)-C(273)	106.6(5)
C(274)-C(272)-C(273)	110.9(6)
O(22)-C(272)-C(275)	102.6(5)
C(274)-C(272)-C(275)	119.2(6)
C(273)-C(272)-C(275)	110.5(6)
C(272)-C(273)-H(27A)	109.5
C(272)-C(273)-H(27B)	109.5
H(27A)-C(273)-H(27B)	109.5
C(272)-C(273)-H(27C)	109.5
H(27A)-C(273)-H(27C)	109.5
H(27B)-C(273)-H(27C)	109.5
C(272)-C(274)-H(27D)	109.5
C(272)-C(274)-H(27E)	109.5
H(27D)-C(274)-H(27E)	109.5
C(272)-C(274)-H(27F)	109.5
H(27D)-C(274)-H(27F)	109.5
H(27E)-C(274)-H(27F)	109.5
N(21)-C(275)-C(276)	107.1(5)
N(21)-C(275)-C(272)	101.8(5)
C(276)-C(275)-C(272)	116.3(6)
N(21)-C(275)-H(27G)	110.4
C(276)-C(275)-H(27G)	110.4
C(272)-C(275)-H(27G)	110.4
C(275)-C(276)-S(21)	110.7(5)
C(275)-C(276)-H(27H)	109.5
S(21)-C(276)-H(27H)	109.5
C(275)-C(276)-H(27I)	109.5
S(21)-C(276)-H(27I)	109.5
H(27H)-C(276)-H(27I)	108.1
Cl(1B)-C(1S)-Cl(2A)	86.3(9)
Cl(1B)-C(1S)-Cl(2B)	107.5(8)
Cl(2A)-C(1S)-Cl(2B)	21.2(6)
Cl(1B)-C(1S)-Cl(2C)	123.8(9)
Cl(2A)-C(1S)-Cl(2C)	37.7(7)
Cl(2B)-C(1S)-Cl(2C)	16.5(5)
Cl(1B)-C(1S)-Cl(1A)	39.5(5)

Cl(2A)-C(1S)-Cl(1A)	101.1(9)
Cl(2B)-C(1S)-Cl(1A)	116.6(9)
Cl(2C)-C(1S)-Cl(1A)	126.9(9)
Cl(1B)-C(1S)-H(1SA)	119.4
Cl(2A)-C(1S)-H(1SA)	34.7
Cl(2B)-C(1S)-H(1SA)	14.6
Cl(2C)-C(1S)-H(1SA)	7.5
Cl(1A)-C(1S)-H(1SA)	119.4
Cl(1B)-C(1S)-H(1SB)	119.4
Cl(2A)-C(1S)-H(1SB)	138.6
Cl(2B)-C(1S)-H(1SB)	123.5
Cl(2C)-C(1S)-H(1SB)	110.5
Cl(1A)-C(1S)-H(1SB)	119.4
H(1SA)-C(1S)-H(1SB)	117.1
Cl(1B)-Cl(1A)-C(1S)	59.7(6)
Cl(1A)-Cl(1B)-C(1S)	80.9(7)
Cl(2B)-Cl(2A)-Cl(2C)	9.5(17)
Cl(2B)-Cl(2A)-C(1S)	82.3(19)
Cl(2C)-Cl(2A)-C(1S)	72.8(10)
Cl(2C)-Cl(2B)-Cl(2A)	158(4)
Cl(2C)-Cl(2B)-C(1S)	82(2)
Cl(2A)-Cl(2B)-C(1S)	76.5(19)
Cl(2B)-Cl(2C)-Cl(2A)	12(2)
Cl(2B)-Cl(2C)-C(1S)	82(2)
Cl(2A)-Cl(2C)-C(1S)	69.5(9)

Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for Δ-**3g** (cla1). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	19(1)	18(1)	19(1)	-1(1)	0(1)	0(1)
P(1)	25(1)	33(1)	35(1)	-1(1)	-5(1)	1(1)
Ru(2)	15(1)	23(1)	25(1)	-2(1)	1(1)	-1(1)
P(2)	42(1)	38(1)	31(1)	-6(1)	4(1)	-10(1)
F(11)	67(4)	108(5)	87(4)	48(4)	14(4)	-18(4)
S(11)	28(1)	42(1)	34(1)	-14(1)	-4(1)	-3(1)
O(11)	26(3)	33(3)	24(3)	7(2)	-3(2)	-7(3)
N(11)	21(3)	18(3)	20(3)	-5(2)	3(3)	-1(3)
F(12)	54(4)	93(4)	54(3)	-40(3)	-21(3)	16(3)
O(12)	39(3)	15(2)	38(3)	0(2)	-6(3)	4(3)
N(12)	24(3)	18(3)	18(3)	2(2)	5(3)	-3(3)
F(13)	30(3)	75(4)	62(3)	-14(3)	-12(3)	20(3)
N(13)	22(3)	25(3)	22(3)	1(3)	1(3)	1(3)
F(14)	52(3)	46(3)	60(3)	10(2)	3(3)	3(3)
N(14)	24(3)	18(3)	24(3)	3(2)	3(3)	3(4)
F(15)	65(4)	43(3)	81(4)	-25(3)	-25(3)	0(3)
N(15)	25(3)	16(3)	28(3)	-3(3)	7(3)	-2(3)
F(16)	45(3)	61(3)	53(3)	8(2)	-3(3)	26(3)
F(21)	78(4)	45(3)	40(3)	2(2)	8(3)	-11(3)
S(21)	47(1)	31(1)	40(1)	-5(1)	9(1)	6(1)
O(21)	18(2)	33(3)	39(3)	-19(2)	1(3)	4(3)
N(21)	19(3)	21(3)	23(3)	-2(2)	-1(3)	-3(3)
F(22)	36(3)	55(3)	79(4)	-19(3)	-5(3)	-7(3)
O(22)	19(2)	34(3)	20(2)	-1(2)	4(2)	-3(3)
N(22)	28(4)	25(4)	32(3)	-7(3)	5(3)	-2(3)
F(23)	60(3)	41(3)	56(3)	-18(2)	6(3)	-7(3)
N(23)	25(3)	34(4)	23(3)	-8(3)	4(3)	-6(4)
F(24)	43(3)	84(4)	51(3)	-19(3)	1(3)	-11(4)
N(24)	18(4)	22(3)	35(3)	-4(3)	3(3)	-3(3)
F(25)	56(3)	42(3)	37(2)	-7(2)	6(2)	-3(3)
N(25)	11(3)	26(3)	38(3)	-1(3)	8(3)	-5(3)
F(26)	92(4)	54(3)	35(3)	5(2)	12(3)	-16(4)
C(111)	11(4)	30(4)	27(4)	5(3)	0(3)	-5(4)

C(112)	49(5)	39(5)	27(4)	-3(4)	-7(4)	-6(5)
C(113)	56(7)	70(7)	21(4)	-9(4)	-17(5)	-11(6)
C(114)	45(5)	39(5)	25(4)	-2(4)	-7(4)	7(5)
C(115)	30(5)	34(5)	34(4)	14(4)	11(4)	5(4)
C(116)	16(4)	24(4)	21(3)	-5(3)	-8(3)	-1(4)
C(121)	25(4)	30(4)	22(4)	-1(3)	1(4)	-4(4)
C(122)	31(5)	33(4)	34(4)	4(4)	7(4)	-9(5)
C(123)	36(5)	36(4)	22(4)	-7(3)	6(4)	10(5)
C(124)	29(4)	22(4)	24(4)	-3(3)	-5(3)	7(4)
C(125)	17(4)	20(3)	29(4)	-1(3)	-3(3)	3(4)
C(131)	33(5)	34(5)	33(4)	4(4)	4(4)	4(5)
C(132)	33(5)	26(4)	44(5)	13(4)	15(4)	-4(4)
C(133)	35(4)	9(3)	70(6)	2(4)	7(6)	-2(4)
C(134)	32(5)	18(4)	47(5)	-1(3)	10(4)	1(4)
C(135)	15(4)	20(4)	25(4)	1(3)	-4(3)	0(3)
C(141)	21(4)	23(4)	36(4)	-2(3)	-4(4)	3(4)
C(142)	25(4)	24(4)	52(5)	14(4)	-9(4)	1(4)
C(143)	41(5)	51(6)	32(5)	5(4)	-14(5)	-12(6)
C(144)	44(5)	38(5)	23(4)	6(3)	-3(4)	-11(5)
C(145)	31(4)	17(4)	30(4)	-3(3)	4(4)	-5(4)
C(151)	25(4)	43(5)	35(4)	1(4)	-1(4)	11(5)
C(152)	26(5)	50(6)	43(5)	7(4)	11(4)	6(5)
C(153)	50(6)	51(6)	52(6)	4(5)	35(6)	12(6)
C(154)	51(6)	33(5)	34(5)	-6(4)	11(5)	-12(5)
C(155)	26(4)	15(4)	20(4)	-1(3)	3(4)	-5(4)
C(160)	29(4)	36(5)	43(5)	5(4)	-9(4)	-4(5)
C(161)	13(4)	42(5)	38(5)	4(4)	5(4)	-5(4)
C(162)	33(5)	44(5)	24(4)	4(4)	-7(4)	-12(5)
C(163)	24(4)	50(6)	41(5)	16(4)	0(4)	-16(5)
C(164)	31(5)	34(5)	52(5)	5(4)	-1(5)	-2(5)
C(165)	43(5)	38(5)	46(5)	-10(4)	0(5)	-1(5)
C(166)	28(4)	69(7)	31(5)	-2(4)	4(4)	-15(5)
C(171)	20(4)	25(4)	35(4)	8(3)	10(4)	3(4)
C(172)	39(5)	20(4)	37(4)	-5(3)	-9(4)	6(4)
C(173)	40(5)	48(6)	50(5)	-11(4)	-6(5)	14(5)
C(174)	61(6)	18(4)	100(7)	2(5)	-37(6)	1(5)
C(175)	17(4)	22(4)	19(3)	-5(3)	1(3)	0(4)
C(176)	27(4)	28(4)	23(4)	0(3)	2(4)	-1(4)
C(211)	24(4)	23(4)	22(4)	-3(3)	-4(4)	-4(4)

C(212)	19(4)	30(4)	30(4)	-4(3)	3(4)	-3(4)
C(213)	41(5)	26(4)	27(4)	-10(3)	-6(4)	-10(4)
C(214)	23(4)	44(5)	37(4)	-9(4)	4(4)	-5(5)
C(215)	22(4)	36(5)	31(4)	-4(4)	4(4)	0(4)
C(216)	15(3)	24(4)	16(3)	2(3)	-2(3)	-6(4)
C(221)	22(4)	37(5)	60(6)	-3(4)	-2(5)	-3(4)
C(222)	19(4)	48(6)	89(8)	0(5)	-13(5)	4(5)
C(223)	22(5)	58(7)	79(7)	-9(6)	21(5)	-11(5)
C(224)	36(5)	56(6)	35(5)	-3(4)	8(5)	-1(5)
C(225)	27(4)	36(5)	31(4)	-12(4)	12(4)	-4(4)
C(231)	24(4)	47(5)	28(4)	-2(4)	-7(4)	-5(4)
C(232)	31(4)	57(6)	23(4)	8(4)	4(4)	10(5)
C(233)	56(6)	78(7)	24(4)	12(4)	-5(5)	11(6)
C(234)	41(5)	82(7)	29(4)	7(5)	10(4)	-37(6)
C(235)	20(4)	41(5)	22(4)	-5(3)	4(4)	-11(4)
C(241)	31(5)	25(4)	31(4)	5(3)	6(4)	7(4)
C(242)	33(5)	20(4)	59(5)	-7(4)	6(5)	-12(5)
C(243)	37(5)	36(5)	46(5)	-20(4)	3(5)	-7(5)
C(244)	34(5)	42(5)	30(4)	-7(4)	-5(4)	2(5)
C(245)	18(4)	26(4)	24(4)	1(3)	3(4)	-1(4)
C(251)	17(4)	27(4)	46(5)	-1(3)	-1(4)	2(4)
C(252)	18(4)	27(4)	65(6)	15(4)	4(5)	2(4)
C(253)	31(5)	47(5)	42(5)	21(4)	6(5)	0(5)
C(254)	32(5)	39(5)	39(4)	12(4)	9(5)	10(5)
C(255)	15(4)	34(4)	21(3)	-1(3)	-2(3)	4(4)
C(260)	47(6)	26(5)	66(6)	-7(4)	4(5)	15(5)
C(261)	42(5)	19(4)	54(5)	9(4)	-8(5)	8(4)
C(262)	49(6)	24(4)	35(5)	5(4)	-15(5)	0(5)
C(263)	63(6)	28(5)	48(5)	14(4)	-20(5)	-6(5)
C(264)	58(6)	45(5)	51(6)	19(4)	-16(6)	-9(6)
C(265)	64(7)	54(6)	84(8)	6(5)	-25(7)	-20(7)
C(266)	71(7)	37(5)	45(5)	-10(4)	-19(5)	5(6)
C(271)	16(4)	27(4)	21(4)	7(3)	-2(3)	-4(4)
C(272)	25(4)	34(4)	13(3)	0(3)	7(3)	9(4)
C(273)	37(4)	33(5)	24(4)	7(3)	11(4)	-10(5)
C(274)	28(4)	32(4)	42(4)	-9(4)	11(4)	4(4)
C(275)	18(4)	20(4)	25(4)	2(3)	5(3)	-4(4)
C(276)	21(4)	29(4)	34(4)	2(4)	4(4)	4(4)
C(1S)	22(7)	36(7)	42(7)	-2(6)	15(6)	-17(7)

Cl(1A)	56(6)	40(5)	81(6)	-49(5)	29(5)	-29(5)
Cl(1B)	43(4)	13(3)	41(4)	-16(3)	6(4)	-15(4)
Cl(2A)	28(7)	59(8)	57(8)	40(6)	-17(6)	-21(7)
Cl(2B)	23(7)	11(7)	27(7)	-25(5)	-10(5)	-2(6)
Cl(2C)	4(5)	27(7)	14(6)	-11(5)	2(5)	-7(5)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for Δ-**3g** (cla1).

	x	y	z	U(eq)
H(11A)	5061	2538	6592	46
H(11B)	4751	3457	6104	59
H(11C)	5011	4996	6127	43
H(11D)	5732	5603	6625	39
H(12A)	8189	3984	7030	31
H(12B)	8813	3584	6476	39
H(12C)	8591	2109	6272	37
H(12D)	7788	1086	6622	30
H(13A)	6178	1503	8065	40
H(13B)	6203	-30	8034	41
H(13C)	6786	-730	7532	45
H(13D)	7360	139	7051	39
H(14A)	8857	2847	7777	32
H(14B)	9739	2893	8291	41
H(14C)	9055	3290	8829	49
H(14D)	7449	3582	8851	42
H(15A)	4667	3312	7697	41
H(15B)	3679	3577	8163	48
H(15C)	4304	3774	8742	62
H(15D)	5894	3719	8821	47
H(16A)	9926	5999	7604	43
H(16B)	10242	6364	7986	43
H(16C)	10704	5177	8451	41
H(16D)	11514	3865	8544	46
H(16E)	11786	2894	8082	47
H(16F)	11217	3196	7515	51
H(16G)	10387	4526	7411	51
H(17A)	5328	6624	7755	69
H(17B)	5879	6170	8080	69
H(17C)	5308	5559	7805	69
H(17D)	6600	7375	7490	89
H(17E)	7535	6859	7379	89
H(17F)	7331	7075	7791	89

H(17G)	7012	5042	7962	23
H(17H)	8321	5509	7420	31
H(17I)	8431	4605	7647	31
H(21A)	7449	1891	9134	31
H(21B)	6248	1174	8849	38
H(21C)	4684	1484	8993	41
H(21D)	4371	2532	9432	36
H(22A)	9361	3805	10154	48
H(22B)	10867	3920	9935	62
H(22C)	11110	4577	9376	64
H(22D)	9857	5192	9071	51
H(23A)	5853	5134	9406	40
H(23B)	5791	5889	8873	44
H(23C)	7156	6258	8584	63
H(23D)	8584	5845	8839	61
H(24A)	7497	6363	9938	35
H(24B)	7794	7417	10365	45
H(24C)	7958	7009	10959	47
H(24D)	7863	5493	11107	42
H(25A)	7442	2324	10186	36
H(25B)	7500	1626	10742	44
H(25C)	7599	2486	11263	48
H(25D)	7699	4048	11208	44
H(26A)	4061	7045	10051	56
H(26B)	4293	7680	10383	56
H(26C)	5171	6960	9545	43
H(26D)	6407	7615	9242	55
H(26E)	7343	8680	9516	62
H(26F)	7052	9097	10105	81
H(26G)	5806	8439	10418	61
H(27A)	4096	2851	10596	47
H(27B)	4716	3553	10815	47
H(27C)	5200	2885	10536	47
H(27D)	3080	3866	10323	51
H(27E)	3436	4698	10090	51
H(27F)	3503	4730	10517	51
H(27G)	5703	4574	10499	25
H(27H)	4681	5489	9946	34
H(27I)	5762	5726	10002	34

H(1SA)	8012	9133	8712	40
H(1SB)	9086	9426	8568	40

Table S6. Torsion angles [°] for Δ-**3g** (cla1).

N(13)-Ru(1)-O(11)-C(111)	-148.9(6)
N(15)-Ru(1)-O(11)-C(111)	113.6(6)
N(14)-Ru(1)-O(11)-C(111)	148.3(15)
N(12)-Ru(1)-O(11)-C(111)	-68.8(6)
N(11)-Ru(1)-O(11)-C(111)	27.0(6)
N(13)-Ru(1)-N(11)-C(171)	30(2)
N(15)-Ru(1)-N(11)-C(171)	-101.7(6)
N(14)-Ru(1)-N(11)-C(171)	179.6(5)
O(11)-Ru(1)-N(11)-C(171)	-7.1(5)
N(12)-Ru(1)-N(11)-C(171)	75.4(6)
N(13)-Ru(1)-N(11)-C(175)	-157.6(18)
N(15)-Ru(1)-N(11)-C(175)	70.7(5)
N(14)-Ru(1)-N(11)-C(175)	-8.1(5)
O(11)-Ru(1)-N(11)-C(175)	165.3(5)
N(12)-Ru(1)-N(11)-C(175)	-112.2(5)
N(13)-Ru(1)-N(12)-C(121)	-175.8(6)
N(15)-Ru(1)-N(12)-C(121)	137(3)
N(14)-Ru(1)-N(12)-C(121)	-87.9(6)
O(11)-Ru(1)-N(12)-C(121)	96.9(6)
N(11)-Ru(1)-N(12)-C(121)	9.1(6)
N(13)-Ru(1)-N(12)-C(125)	18.6(5)
N(15)-Ru(1)-N(12)-C(125)	-29(4)
N(14)-Ru(1)-N(12)-C(125)	106.5(5)
O(11)-Ru(1)-N(12)-C(125)	-68.7(5)
N(11)-Ru(1)-N(12)-C(125)	-156.5(5)
N(15)-Ru(1)-N(13)-C(135)	162.8(5)
N(14)-Ru(1)-N(13)-C(135)	-118.1(5)
O(11)-Ru(1)-N(13)-C(135)	68.8(5)
N(12)-Ru(1)-N(13)-C(135)	-14.5(5)
N(11)-Ru(1)-N(13)-C(135)	32(2)
N(15)-Ru(1)-N(13)-C(131)	-14.3(7)
N(14)-Ru(1)-N(13)-C(131)	64.8(6)
O(11)-Ru(1)-N(13)-C(131)	-108.3(6)
N(12)-Ru(1)-N(13)-C(131)	168.4(7)
N(11)-Ru(1)-N(13)-C(131)	-145.5(18)
N(13)-Ru(1)-N(14)-C(141)	75.7(6)
N(15)-Ru(1)-N(14)-C(141)	173.6(7)

O(11)-Ru(1)-N(14)-C(141)	138.2(15)
N(12)-Ru(1)-N(14)-C(141)	-3.8(7)
N(11)-Ru(1)-N(14)-C(141)	-100.8(6)
N(13)-Ru(1)-N(14)-C(145)	-101.2(5)
N(15)-Ru(1)-N(14)-C(145)	-3.3(5)
O(11)-Ru(1)-N(14)-C(145)	-38.7(19)
N(12)-Ru(1)-N(14)-C(145)	179.3(5)
N(11)-Ru(1)-N(14)-C(145)	82.2(5)
N(13)-Ru(1)-N(15)-C(151)	-88.6(7)
N(14)-Ru(1)-N(15)-C(151)	-177.5(7)
O(11)-Ru(1)-N(15)-C(151)	-2.1(7)
N(12)-Ru(1)-N(15)-C(151)	-42(4)
N(11)-Ru(1)-N(15)-C(151)	86.3(7)
N(13)-Ru(1)-N(15)-C(155)	92.1(5)
N(14)-Ru(1)-N(15)-C(155)	3.2(5)
O(11)-Ru(1)-N(15)-C(155)	178.6(5)
N(12)-Ru(1)-N(15)-C(155)	139(3)
N(11)-Ru(1)-N(15)-C(155)	-93.0(5)
N(22)-Ru(2)-O(21)-C(211)	-160.4(6)
N(25)-Ru(2)-O(21)-C(211)	100.0(6)
N(24)-Ru(2)-O(21)-C(211)	136.3(13)
N(23)-Ru(2)-O(21)-C(211)	-81.6(6)
N(21)-Ru(2)-O(21)-C(211)	15.2(6)
N(22)-Ru(2)-N(21)-C(271)	37(2)
N(25)-Ru(2)-N(21)-C(271)	-102.0(6)
N(24)-Ru(2)-N(21)-C(271)	180.0(6)
O(21)-Ru(2)-N(21)-C(271)	-7.9(6)
N(23)-Ru(2)-N(21)-C(271)	79.5(6)
N(22)-Ru(2)-N(21)-C(275)	-147(2)
N(25)-Ru(2)-N(21)-C(275)	74.0(5)
N(24)-Ru(2)-N(21)-C(275)	-4.0(5)
O(21)-Ru(2)-N(21)-C(275)	168.1(5)
N(23)-Ru(2)-N(21)-C(275)	-104.5(5)
N(25)-Ru(2)-N(22)-C(221)	2.4(7)
N(24)-Ru(2)-N(22)-C(221)	80.8(6)
O(21)-Ru(2)-N(22)-C(221)	-91.0(6)
N(23)-Ru(2)-N(22)-C(221)	-179.2(7)
N(21)-Ru(2)-N(22)-C(221)	-136(2)
N(25)-Ru(2)-N(22)-C(225)	176.5(5)

N(24)-Ru(2)-N(22)-C(225)	-105.1(5)
O(21)-Ru(2)-N(22)-C(225)	83.1(5)
N(23)-Ru(2)-N(22)-C(225)	-5.1(5)
N(21)-Ru(2)-N(22)-C(225)	38(2)
N(22)-Ru(2)-N(23)-C(231)	179.6(7)
N(25)-Ru(2)-N(23)-C(231)	-132(7)
N(24)-Ru(2)-N(23)-C(231)	-92.7(7)
O(21)-Ru(2)-N(23)-C(231)	93.0(6)
N(21)-Ru(2)-N(23)-C(231)	3.9(7)
N(22)-Ru(2)-N(23)-C(235)	2.4(5)
N(25)-Ru(2)-N(23)-C(235)	51(7)
N(24)-Ru(2)-N(23)-C(235)	90.1(5)
O(21)-Ru(2)-N(23)-C(235)	-84.2(5)
N(21)-Ru(2)-N(23)-C(235)	-173.3(5)
N(22)-Ru(2)-N(24)-C(245)	-100.8(6)
N(25)-Ru(2)-N(24)-C(245)	-0.8(5)
O(21)-Ru(2)-N(24)-C(245)	-37.9(17)
N(23)-Ru(2)-N(24)-C(245)	-179.4(6)
N(21)-Ru(2)-N(24)-C(245)	82.9(6)
N(22)-Ru(2)-N(24)-C(241)	73.4(7)
N(25)-Ru(2)-N(24)-C(241)	173.5(7)
O(21)-Ru(2)-N(24)-C(241)	136.4(12)
N(23)-Ru(2)-N(24)-C(241)	-5.1(7)
N(21)-Ru(2)-N(24)-C(241)	-102.8(7)
N(22)-Ru(2)-N(25)-C(251)	-96.0(7)
N(24)-Ru(2)-N(25)-C(251)	176.3(7)
O(21)-Ru(2)-N(25)-C(251)	-9.2(7)
N(23)-Ru(2)-N(25)-C(251)	-144(6)
N(21)-Ru(2)-N(25)-C(251)	79.8(7)
N(22)-Ru(2)-N(25)-C(255)	91.9(5)
N(24)-Ru(2)-N(25)-C(255)	4.2(5)
O(21)-Ru(2)-N(25)-C(255)	178.7(5)
N(23)-Ru(2)-N(25)-C(255)	44(7)
N(21)-Ru(2)-N(25)-C(255)	-92.3(5)
Ru(1)-O(11)-C(111)-C(116)	-30.3(10)
Ru(1)-O(11)-C(111)-C(112)	153.9(5)
O(11)-C(111)-C(112)-C(113)	176.9(8)
C(116)-C(111)-C(112)-C(113)	0.7(11)
C(111)-C(112)-C(113)-C(114)	-2.5(14)

C(112)-C(113)-C(114)-C(115)	3.1(15)
C(113)-C(114)-C(115)-C(116)	-2.0(13)
C(114)-C(115)-C(116)-C(111)	0.3(12)
C(114)-C(115)-C(116)-C(171)	179.3(7)
O(11)-C(111)-C(116)-C(115)	-175.4(7)
C(112)-C(111)-C(116)-C(115)	0.4(11)
O(11)-C(111)-C(116)-C(171)	5.6(12)
C(112)-C(111)-C(116)-C(171)	-178.6(7)
C(125)-N(12)-C(121)-C(122)	2.3(11)
Ru(1)-N(12)-C(121)-C(122)	-162.5(6)
N(12)-C(121)-C(122)-C(123)	0.1(11)
C(121)-C(122)-C(123)-C(124)	-0.8(12)
C(122)-C(123)-C(124)-C(125)	-0.8(11)
C(121)-N(12)-C(125)-C(124)	-4.0(10)
Ru(1)-N(12)-C(125)-C(124)	163.0(5)
C(121)-N(12)-C(125)-C(135)	173.2(6)
Ru(1)-N(12)-C(125)-C(135)	-19.8(7)
C(123)-C(124)-C(125)-N(12)	3.2(10)
C(123)-C(124)-C(125)-C(135)	-173.7(7)
C(135)-N(13)-C(131)-C(132)	0.6(12)
Ru(1)-N(13)-C(131)-C(132)	177.6(7)
N(13)-C(131)-C(132)-C(133)	-1.0(14)
C(131)-C(132)-C(133)-C(134)	0.1(13)
C(132)-C(133)-C(134)-C(135)	1.0(12)
C(131)-N(13)-C(135)-C(134)	0.7(10)
Ru(1)-N(13)-C(135)-C(134)	-176.8(6)
C(131)-N(13)-C(135)-C(125)	-174.5(6)
Ru(1)-N(13)-C(135)-C(125)	8.0(7)
C(133)-C(134)-C(135)-N(13)	-1.5(12)
C(133)-C(134)-C(135)-C(125)	173.3(7)
N(12)-C(125)-C(135)-N(13)	8.1(9)
C(124)-C(125)-C(135)-N(13)	-174.8(6)
N(12)-C(125)-C(135)-C(134)	-167.1(7)
C(124)-C(125)-C(135)-C(134)	10.0(11)
C(145)-N(14)-C(141)-C(142)	-1.2(11)
Ru(1)-N(14)-C(141)-C(142)	-178.0(5)
N(14)-C(141)-C(142)-C(143)	-0.8(12)
C(141)-C(142)-C(143)-C(144)	1.6(13)
C(142)-C(143)-C(144)-C(145)	-0.4(13)

C(141)-N(14)-C(145)-C(144)	2.4(10)
Ru(1)-N(14)-C(145)-C(144)	179.6(5)
C(141)-N(14)-C(145)-C(155)	-174.2(7)
Ru(1)-N(14)-C(145)-C(155)	3.1(8)
C(143)-C(144)-C(145)-N(14)	-1.6(12)
C(143)-C(144)-C(145)-C(155)	174.5(8)
C(155)-N(15)-C(151)-C(152)	-0.5(12)
Ru(1)-N(15)-C(151)-C(152)	-179.8(6)
N(15)-C(151)-C(152)-C(153)	0.1(14)
C(151)-C(152)-C(153)-C(154)	0.6(14)
C(152)-C(153)-C(154)-C(155)	-0.8(14)
C(151)-N(15)-C(155)-C(154)	0.3(11)
Ru(1)-N(15)-C(155)-C(154)	179.6(6)
C(151)-N(15)-C(155)-C(145)	178.2(7)
Ru(1)-N(15)-C(155)-C(145)	-2.4(8)
C(153)-C(154)-C(155)-N(15)	0.3(13)
C(153)-C(154)-C(155)-C(145)	-177.4(8)
N(14)-C(145)-C(155)-N(15)	-0.4(10)
C(144)-C(145)-C(155)-N(15)	-176.8(6)
N(14)-C(145)-C(155)-C(154)	177.4(6)
C(144)-C(145)-C(155)-C(154)	1.1(13)
C(176)-S(11)-C(160)-C(161)	-78.4(6)
S(11)-C(160)-C(161)-C(162)	-78.0(9)
S(11)-C(160)-C(161)-C(166)	102.1(8)
C(166)-C(161)-C(162)-C(163)	-0.1(11)
C(160)-C(161)-C(162)-C(163)	180.0(7)
C(161)-C(162)-C(163)-C(164)	0.5(12)
C(162)-C(163)-C(164)-C(165)	-0.8(12)
C(163)-C(164)-C(165)-C(166)	0.7(13)
C(164)-C(165)-C(166)-C(161)	-0.4(12)
C(162)-C(161)-C(166)-C(165)	0.0(11)
C(160)-C(161)-C(166)-C(165)	180.0(7)
C(175)-N(11)-C(171)-O(12)	-3.8(8)
Ru(1)-N(11)-C(171)-O(12)	169.9(5)
C(175)-N(11)-C(171)-C(116)	174.6(7)
Ru(1)-N(11)-C(171)-C(116)	-11.7(10)
C(172)-O(12)-C(171)-N(11)	-13.3(8)
C(172)-O(12)-C(171)-C(116)	168.1(6)
C(115)-C(116)-C(171)-N(11)	-161.6(7)

C(111)-C(116)-C(171)-N(11)	17.4(11)
C(115)-C(116)-C(171)-O(12)	16.8(10)
C(111)-C(116)-C(171)-O(12)	-164.2(7)
C(171)-O(12)-C(172)-C(173)	-94.3(7)
C(171)-O(12)-C(172)-C(174)	146.2(6)
C(171)-O(12)-C(172)-C(175)	23.0(7)
C(171)-N(11)-C(175)-C(176)	-109.1(6)
Ru(1)-N(11)-C(175)-C(176)	77.5(7)
C(171)-N(11)-C(175)-C(172)	17.8(7)
Ru(1)-N(11)-C(175)-C(172)	-155.7(5)
O(12)-C(172)-C(175)-N(11)	-24.1(6)
C(173)-C(172)-C(175)-N(11)	90.1(7)
C(174)-C(172)-C(175)-N(11)	-139.7(7)
O(12)-C(172)-C(175)-C(176)	95.9(7)
C(173)-C(172)-C(175)-C(176)	-149.9(7)
C(174)-C(172)-C(175)-C(176)	-19.8(10)
N(11)-C(175)-C(176)-S(11)	-164.3(4)
C(172)-C(175)-C(176)-S(11)	79.6(7)
C(160)-S(11)-C(176)-C(175)	-175.2(5)
Ru(2)-O(21)-C(211)-C(216)	-10.2(10)
Ru(2)-O(21)-C(211)-C(212)	169.0(4)
O(21)-C(211)-C(212)-C(213)	-176.2(7)
C(216)-C(211)-C(212)-C(213)	3.1(10)
C(211)-C(212)-C(213)-C(214)	-1.8(11)
C(212)-C(213)-C(214)-C(215)	-0.3(12)
C(213)-C(214)-C(215)-C(216)	1.0(12)
C(214)-C(215)-C(216)-C(211)	0.4(11)
C(214)-C(215)-C(216)-C(271)	-175.9(7)
O(21)-C(211)-C(216)-C(215)	176.8(7)
C(212)-C(211)-C(216)-C(215)	-2.4(10)
O(21)-C(211)-C(216)-C(271)	-6.8(11)
C(212)-C(211)-C(216)-C(271)	173.9(6)
C(225)-N(22)-C(221)-C(222)	0.2(12)
Ru(2)-N(22)-C(221)-C(222)	174.2(7)
N(22)-C(221)-C(222)-C(223)	-1.2(14)
C(221)-C(222)-C(223)-C(224)	2.2(14)
C(222)-C(223)-C(224)-C(225)	-2.2(14)
C(221)-N(22)-C(225)-C(224)	-0.3(11)
Ru(2)-N(22)-C(225)-C(224)	-174.8(6)

C(221)-N(22)-C(225)-C(235)	-178.5(7)
Ru(2)-N(22)-C(225)-C(235)	7.0(9)
C(223)-C(224)-C(225)-N(22)	1.3(13)
C(223)-C(224)-C(225)-C(235)	179.3(8)
C(235)-N(23)-C(231)-C(232)	-0.5(12)
Ru(2)-N(23)-C(231)-C(232)	-177.6(6)
N(23)-C(231)-C(232)-C(233)	-1.6(14)
C(231)-C(232)-C(233)-C(234)	0.6(14)
C(232)-C(233)-C(234)-C(235)	2.4(15)
C(231)-N(23)-C(235)-C(234)	3.5(11)
Ru(2)-N(23)-C(235)-C(234)	-179.0(6)
C(231)-N(23)-C(235)-C(225)	-176.9(7)
Ru(2)-N(23)-C(235)-C(225)	0.5(8)
C(233)-C(234)-C(235)-N(23)	-4.5(13)
C(233)-C(234)-C(235)-C(225)	176.0(8)
N(22)-C(225)-C(235)-N(23)	-4.9(10)
C(224)-C(225)-C(235)-N(23)	177.0(7)
N(22)-C(225)-C(235)-C(234)	174.6(8)
C(224)-C(225)-C(235)-C(234)	-3.5(13)
C(245)-N(24)-C(241)-C(242)	-0.5(12)
Ru(2)-N(24)-C(241)-C(242)	-174.7(6)
N(24)-C(241)-C(242)-C(243)	-0.9(13)
C(241)-C(242)-C(243)-C(244)	1.2(13)
C(242)-C(243)-C(244)-C(245)	-0.1(13)
C(241)-N(24)-C(245)-C(244)	1.5(12)
Ru(2)-N(24)-C(245)-C(244)	176.4(6)
C(241)-N(24)-C(245)-C(255)	-177.3(7)
Ru(2)-N(24)-C(245)-C(255)	-2.5(9)
C(243)-C(244)-C(245)-N(24)	-1.3(13)
C(243)-C(244)-C(245)-C(255)	177.5(8)
C(255)-N(25)-C(251)-C(252)	-1.2(12)
Ru(2)-N(25)-C(251)-C(252)	-173.1(5)
N(25)-C(251)-C(252)-C(253)	0.9(13)
C(251)-C(252)-C(253)-C(254)	-1.0(13)
C(252)-C(253)-C(254)-C(255)	1.6(14)
C(251)-N(25)-C(255)-C(254)	1.8(12)
Ru(2)-N(25)-C(255)-C(254)	174.4(6)
C(251)-N(25)-C(255)-C(245)	-179.4(7)
Ru(2)-N(25)-C(255)-C(245)	-6.8(9)

C(253)-C(254)-C(255)-N(25)	-2.0(13)
C(253)-C(254)-C(255)-C(245)	179.2(8)
N(24)-C(245)-C(255)-N(25)	6.1(10)
C(244)-C(245)-C(255)-N(25)	-172.8(7)
N(24)-C(245)-C(255)-C(254)	-175.1(7)
C(244)-C(245)-C(255)-C(254)	6.0(13)
C(276)-S(21)-C(260)-C(261)	-65.4(7)
S(21)-C(260)-C(261)-C(262)	93.0(9)
S(21)-C(260)-C(261)-C(266)	-86.8(8)
C(266)-C(261)-C(262)-C(263)	-0.2(12)
C(260)-C(261)-C(262)-C(263)	-180.0(7)
C(261)-C(262)-C(263)-C(264)	-0.1(12)
C(262)-C(263)-C(264)-C(265)	0.2(13)
C(263)-C(264)-C(265)-C(266)	-0.1(14)
C(262)-C(261)-C(266)-C(265)	0.4(12)
C(260)-C(261)-C(266)-C(265)	-179.9(8)
C(264)-C(265)-C(266)-C(261)	-0.2(14)
C(275)-N(21)-C(271)-O(22)	-0.5(8)
Ru(2)-N(21)-C(271)-O(22)	176.1(4)
C(275)-N(21)-C(271)-C(216)	178.6(7)
Ru(2)-N(21)-C(271)-C(216)	-4.8(10)
C(272)-O(22)-C(271)-N(21)	-14.2(8)
C(272)-O(22)-C(271)-C(216)	166.6(5)
C(215)-C(216)-C(271)-N(21)	-168.3(7)
C(211)-C(216)-C(271)-N(21)	15.3(11)
C(215)-C(216)-C(271)-O(22)	10.8(9)
C(211)-C(216)-C(271)-O(22)	-165.6(6)
C(271)-O(22)-C(272)-C(274)	147.2(6)
C(271)-O(22)-C(272)-C(273)	-94.6(6)
C(271)-O(22)-C(272)-C(275)	21.5(6)
C(271)-N(21)-C(275)-C(276)	-108.4(6)
Ru(2)-N(21)-C(275)-C(276)	75.1(7)
C(271)-N(21)-C(275)-C(272)	14.2(7)
Ru(2)-N(21)-C(275)-C(272)	-162.3(4)
O(22)-C(272)-C(275)-N(21)	-21.0(6)
C(274)-C(272)-C(275)-N(21)	-137.6(6)
C(273)-C(272)-C(275)-N(21)	92.3(6)
O(22)-C(272)-C(275)-C(276)	95.0(7)
C(274)-C(272)-C(275)-C(276)	-21.6(9)

C(273)-C(272)-C(275)-C(276)	-151.7(6)
N(21)-C(275)-C(276)-S(21)	-158.7(4)
C(272)-C(275)-C(276)-S(21)	88.3(6)
C(260)-S(21)-C(276)-C(275)	-171.4(5)
Cl(2A)-C(1S)-Cl(1A)-Cl(1B)	70.0(10)
Cl(2B)-C(1S)-Cl(1A)-Cl(1B)	85.4(11)
Cl(2C)-C(1S)-Cl(1A)-Cl(1B)	100.6(12)
Cl(2A)-C(1S)-Cl(1B)-Cl(1A)	-112.5(9)
Cl(2B)-C(1S)-Cl(1B)-Cl(1A)	-110.9(11)
Cl(2C)-C(1S)-Cl(1B)-Cl(1A)	-108.8(12)
Cl(1B)-C(1S)-Cl(2A)-Cl(2B)	176(2)
Cl(2C)-C(1S)-Cl(2A)-Cl(2B)	1(2)
Cl(1A)-C(1S)-Cl(2A)-Cl(2B)	139(2)
Cl(1B)-C(1S)-Cl(2A)-Cl(2C)	175.0(12)
Cl(2B)-C(1S)-Cl(2A)-Cl(2C)	-1(2)
Cl(1A)-C(1S)-Cl(2A)-Cl(2C)	138.2(12)
C(1S)-Cl(2A)-Cl(2B)-Cl(2C)	-5(13)
Cl(2C)-Cl(2A)-Cl(2B)-C(1S)	5(13)
Cl(1B)-C(1S)-Cl(2B)-Cl(2C)	174(3)
Cl(2A)-C(1S)-Cl(2B)-Cl(2C)	178(5)
Cl(1A)-C(1S)-Cl(2B)-Cl(2C)	132(3)
Cl(1B)-C(1S)-Cl(2B)-Cl(2A)	-4(2)
Cl(2C)-C(1S)-Cl(2B)-Cl(2A)	-178(5)
Cl(1A)-C(1S)-Cl(2B)-Cl(2A)	-46(2)
C(1S)-Cl(2B)-Cl(2C)-Cl(2A)	-5(13)
Cl(2A)-Cl(2B)-Cl(2C)-C(1S)	5(13)
C(1S)-Cl(2A)-Cl(2C)-Cl(2B)	175(13)
Cl(2B)-Cl(2A)-Cl(2C)-C(1S)	-175(13)
Cl(1B)-C(1S)-Cl(2C)-Cl(2B)	-7(4)
Cl(2A)-C(1S)-Cl(2C)-Cl(2B)	-1(3)
Cl(1A)-C(1S)-Cl(2C)-Cl(2B)	-56(3)
Cl(1B)-C(1S)-Cl(2C)-Cl(2A)	-6.1(15)
Cl(2B)-C(1S)-Cl(2C)-Cl(2A)	1(3)
Cl(1A)-C(1S)-Cl(2C)-Cl(2A)	-54.8(14)

Crystals of Δ-**5** (as BPh_4 salt) were obtained by slow diffusion from a solution in actone layered with Et_2O. Data were collected on an Oxford Xcalibur, Sapphire3, Gemini ultra detector employing graphite-monochromated Mo-K_α radiation (λ = 0.71073 Å) at a temperature of 100 K. The structure was solved by SHELXS-97. Refinement was done by full-matrix least squares based on F^2 data of one twin domain using SHELXL-97. The absolute configuration was determined. The detailed information is listed in the Tables S7-S12.

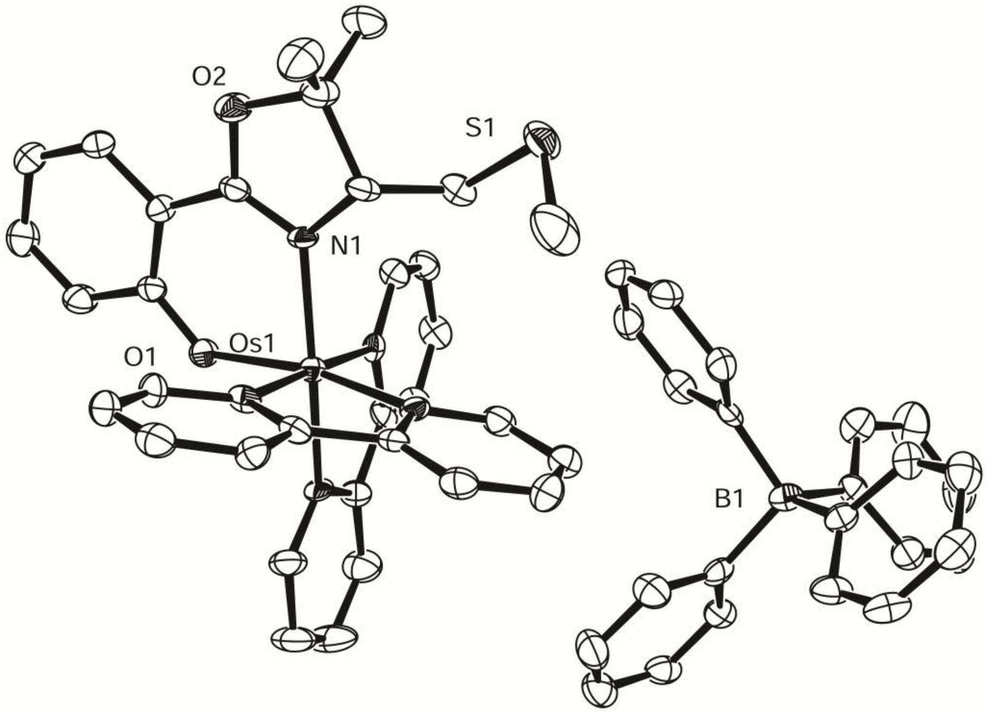


Figure S19. ORTEP drawing of compound Δ-**5** (BPh_4 counterion) with 50% probability thermal ellipsoids.

Table S7. Crystal data and structure refinement for Δ-**5** (BPh_4).

Identification code	dxb	
Empirical formula	C57 H52 B N5 O2 Os S	
Formula weight	1072.11	
Temperature	163(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 9.4352(19) Å	α= 90°.
	b = 19.433(4) Å	β= 90°.
	c = 25.513(5) Å	γ = 90°.
Volume	4677.9(16) $Å^3$	
Z	4	
Density (calculated)	1.522 Mg/m^3	
Absorption coefficient	2.821 mm^{-1}	
F(000)	2168	
Crystal size	0.28 x 0.20 x 0.18 mm^3	
Theta range for data collection	1.32 to 26.00°.	
Index ranges	-11<=h<=11, -23<=k<=23, -31<=l<=31	
Reflections collected	36663	
Independent reflections	9190 [R(int) = 0.0529]	
Completeness to theta = 26.00°	99.9 %	
Absorption correction	Empirical	
Max. and min. transmission	0.6307 and 0.5056	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9190 / 0 / 604	
Goodness-of-fit on F^2	1.001	
Final R indices [I>2sigma(I)]	R1 = 0.0363, wR2 = 0.0777	
R indices (all data)	R1 = 0.0398, wR2 = 0.0788	
Absolute structure parameter	-0.005(7)	
Largest diff. peak and hole	1.698 and -0.783 e.$Å^{-3}$	

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for Δ-**5** (BPh_4). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Os(1)	1366(1)	5344(1)	1073(1)	18(1)
S(1)	5182(2)	4646(1)	-338(1)	35(1)
O(1)	-604(3)	5790(2)	1020(2)	23(1)
O(2)	1488(4)	6297(2)	-418(1)	29(1)
N(1)	1747(4)	5650(2)	297(2)	19(1)
N(2)	3341(5)	4988(2)	1261(2)	20(1)
N(3)	2365(5)	6231(2)	1287(2)	19(1)
N(4)	764(5)	5007(2)	1802(2)	20(1)
N(5)	318(4)	4453(2)	891(2)	16(1)
C(11)	-1129(6)	6178(3)	652(2)	21(1)
C(12)	-2464(6)	6476(3)	742(2)	29(1)
C(13)	-3112(6)	6885(3)	387(2)	34(2)
C(14)	-2459(7)	7035(3)	-92(2)	33(2)
C(15)	-1143(6)	6766(3)	-189(2)	26(1)
C(16)	-436(6)	6340(3)	172(2)	21(1)
C(21)	3725(7)	4316(3)	1291(2)	27(1)
C(22)	5005(6)	4112(3)	1496(2)	28(1)
C(23)	5950(6)	4602(3)	1677(2)	33(1)
C(24)	5570(6)	5275(3)	1661(2)	27(1)
C(25)	4274(6)	5465(3)	1453(2)	20(1)
C(31)	1766(6)	6861(3)	1281(2)	26(1)
C(32)	2514(7)	7444(3)	1406(2)	30(1)
C(33)	3935(6)	7386(3)	1556(2)	29(1)
C(34)	4521(6)	6748(3)	1584(2)	23(1)
C(35)	3757(6)	6176(3)	1440(2)	20(1)
C(41)	1059(6)	5328(3)	2254(2)	30(1)
C(42)	604(8)	5074(3)	2733(2)	40(2)
C(43)	-143(8)	4479(4)	2747(3)	47(2)
C(44)	-440(7)	4142(3)	2285(2)	37(2)
C(45)	18(6)	4414(3)	1820(2)	23(1)
C(51)	34(6)	4215(3)	405(2)	23(1)
C(52)	-780(6)	3656(3)	312(2)	27(1)
C(53)	-1353(8)	3295(3)	726(2)	30(1)

C(54)	-1122(6)	3527(3)	1223(2)	30(1)
C(55)	-280(6)	4106(3)	1304(2)	23(1)
C(61)	953(6)	6072(3)	38(2)	21(1)
C(62)	2823(6)	5932(3)	-523(2)	28(1)
C(63)	3083(6)	5548(3)	6(2)	23(1)
C(64)	3450(6)	4791(3)	-52(2)	26(1)
C(65)	6305(8)	4859(4)	199(3)	55(2)
C(66)	3962(7)	6460(3)	-631(3)	42(2)
C(67)	2500(8)	5484(3)	-992(2)	45(2)
C(111)	3907(5)	2054(3)	1117(2)	22(1)
C(112)	2479(6)	2027(3)	968(2)	30(1)
C(113)	1915(7)	2421(3)	573(2)	38(2)
C(114)	2755(8)	2873(3)	302(2)	36(2)
C(115)	4163(7)	2931(3)	429(2)	32(2)
C(116)	4727(7)	2521(3)	833(2)	29(1)
C(121)	4276(6)	771(3)	1535(2)	27(1)
C(122)	3587(6)	466(3)	1119(2)	37(1)
C(123)	3402(7)	-246(3)	1085(3)	50(2)
C(124)	3904(8)	-662(3)	1479(3)	51(2)
C(125)	4610(7)	-379(4)	1895(3)	44(2)
C(126)	4800(6)	319(3)	1916(2)	34(1)
C(131)	3511(6)	1868(3)	2127(2)	24(1)
C(132)	3514(7)	2559(3)	2266(2)	33(1)
C(133)	2688(7)	2813(4)	2674(3)	42(2)
C(134)	1833(7)	2373(4)	2957(3)	38(2)
C(135)	1805(6)	1687(3)	2823(2)	31(1)
C(136)	2630(6)	1442(3)	2413(2)	26(1)
C(141)	6191(6)	1741(3)	1703(2)	27(1)
C(142)	7155(6)	1512(3)	1323(2)	32(1)
C(143)	8591(7)	1595(3)	1370(2)	35(1)
C(144)	9175(7)	1905(3)	1808(3)	35(2)
C(145)	8263(7)	2126(3)	2188(2)	34(2)
C(146)	6795(6)	2054(3)	2132(2)	33(2)
B(1)	4482(7)	1604(4)	1615(3)	27(2)

Table S9. Bond lengths [Å] and angles [°] for Δ-**5** (BPh_4).

Os(1)-N(3)	2.041(4)
Os(1)-N(2)	2.045(4)
Os(1)-N(5)	2.047(4)
Os(1)-N(4)	2.051(4)
Os(1)-O(1)	2.056(3)
Os(1)-N(1)	2.098(4)
S(1)-C(65)	1.779(7)
S(1)-C(64)	1.811(6)
O(1)-C(11)	1.301(6)
O(2)-C(61)	1.341(6)
O(2)-C(62)	1.470(7)
N(1)-C(61)	1.293(6)
N(1)-C(63)	1.477(7)
N(2)-C(21)	1.359(7)
N(2)-C(25)	1.368(7)
N(3)-C(31)	1.347(7)
N(3)-C(35)	1.374(7)
N(4)-C(41)	1.342(7)
N(4)-C(45)	1.351(7)
N(5)-C(51)	1.351(7)
N(5)-C(55)	1.371(7)
C(11)-C(12)	1.406(8)
C(11)-C(16)	1.424(7)
C(12)-C(13)	1.349(8)
C(12)-H(12A)	0.9500
C(13)-C(14)	1.399(8)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.370(8)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.405(7)
C(15)-H(15A)	0.9500
C(16)-C(61)	1.452(7)
C(21)-C(22)	1.374(9)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.383(8)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.356(8)

C(23)-H(23A)	0.9500
C(24)-C(25)	1.384(7)
C(24)-H(24A)	0.9500
C(25)-C(35)	1.466(7)
C(31)-C(32)	1.373(7)
C(31)-H(31A)	0.9500
C(32)-C(33)	1.399(8)
C(32)-H(32A)	0.9500
C(33)-C(34)	1.360(8)
C(33)-H(33A)	0.9500
C(34)-C(35)	1.374(7)
C(34)-H(34A)	0.9500
C(41)-C(42)	1.385(8)
C(41)-H(41A)	0.9500
C(42)-C(43)	1.355(9)
C(42)-H(42A)	0.9500
C(43)-C(44)	1.375(9)
C(43)-H(43A)	0.9500
C(44)-C(45)	1.371(8)
C(44)-H(44A)	0.9500
C(45)-C(55)	1.473(8)
C(51)-C(52)	1.351(7)
C(51)-H(51A)	0.9500
C(52)-C(53)	1.379(8)
C(52)-H(52A)	0.9500
C(53)-C(54)	1.365(8)
C(53)-H(53A)	0.9500
C(54)-C(55)	1.392(8)
C(54)-H(54A)	0.9500
C(62)-C(67)	1.511(8)
C(62)-C(66)	1.511(8)
C(62)-C(63)	1.562(7)
C(63)-C(64)	1.518(7)
C(63)-H(63A)	1.0000
C(64)-H(64A)	0.9900
C(64)-H(64B)	0.9900
C(65)-H(65A)	0.9800
C(65)-H(65B)	0.9800
C(65)-H(65C)	0.9800

C(66)-H(66A)	0.9800
C(66)-H(66B)	0.9800
C(66)-H(66C)	0.9800
C(67)-H(67A)	0.9800
C(67)-H(67B)	0.9800
C(67)-H(67C)	0.9800
C(111)-C(116)	1.396(8)
C(111)-C(112)	1.400(8)
C(111)-B(1)	1.635(8)
C(112)-C(113)	1.372(8)
C(112)-H(11A)	0.9500
C(113)-C(114)	1.371(9)
C(113)-H(11B)	0.9500
C(114)-C(115)	1.372(9)
C(114)-H(11C)	0.9500
C(115)-C(116)	1.406(8)
C(115)-H(11D)	0.9500
C(116)-H(11E)	0.9500
C(121)-C(122)	1.379(8)
C(121)-C(126)	1.400(8)
C(121)-B(1)	1.643(9)
C(122)-C(123)	1.396(8)
C(122)-H(12B)	0.9500
C(123)-C(124)	1.375(10)
C(123)-H(12C)	0.9500
C(124)-C(125)	1.369(10)
C(124)-H(12D)	0.9500
C(125)-C(126)	1.370(9)
C(125)-H(12E)	0.9500
C(126)-H(12F)	0.9500
C(131)-C(136)	1.383(8)
C(131)-C(132)	1.390(8)
C(131)-B(1)	1.676(9)
C(132)-C(133)	1.390(8)
C(132)-H(13B)	0.9500
C(133)-C(134)	1.379(9)
C(133)-H(13C)	0.9500
C(134)-C(135)	1.375(9)
C(134)-H(13D)	0.9500

C(135)-C(136)	1.388(8)
C(135)-H(13E)	0.9500
C(136)-H(13F)	0.9500
C(141)-C(146)	1.375(8)
C(141)-C(142)	1.403(8)
C(141)-B(1)	1.650(9)
C(142)-C(143)	1.370(9)
C(142)-H(14B)	0.9500
C(143)-C(144)	1.384(9)
C(143)-H(14C)	0.9500
C(144)-C(145)	1.365(9)
C(144)-H(14D)	0.9500
C(145)-C(146)	1.400(8)
C(145)-H(14E)	0.9500
C(146)-H(14F)	0.9500

N(3)-Os(1)-N(2)	78.55(18)
N(3)-Os(1)-N(5)	177.30(17)
N(2)-Os(1)-N(5)	101.99(17)
N(3)-Os(1)-N(4)	98.87(18)
N(2)-Os(1)-N(4)	86.08(17)
N(5)-Os(1)-N(4)	78.55(17)
N(3)-Os(1)-O(1)	94.50(16)
N(2)-Os(1)-O(1)	169.16(16)
N(5)-Os(1)-O(1)	84.57(15)
N(4)-Os(1)-O(1)	86.81(16)
N(3)-Os(1)-N(1)	86.20(17)
N(2)-Os(1)-N(1)	99.28(17)
N(5)-Os(1)-N(1)	96.30(17)
N(4)-Os(1)-N(1)	173.30(18)
O(1)-Os(1)-N(1)	88.44(16)
C(65)-S(1)-C(64)	101.1(3)
C(11)-O(1)-Os(1)	129.5(3)
C(61)-O(2)-C(62)	108.8(4)
C(61)-N(1)-C(63)	108.8(4)
C(61)-N(1)-Os(1)	124.3(3)
C(63)-N(1)-Os(1)	125.6(3)
C(21)-N(2)-C(25)	117.3(5)
C(21)-N(2)-Os(1)	125.5(4)

C(25)-N(2)-Os(1)	116.2(3)
C(31)-N(3)-C(35)	118.4(4)
C(31)-N(3)-Os(1)	124.8(4)
C(35)-N(3)-Os(1)	116.8(3)
C(41)-N(4)-C(45)	118.4(5)
C(41)-N(4)-Os(1)	125.1(4)
C(45)-N(4)-Os(1)	116.5(4)
C(51)-N(5)-C(55)	117.1(4)
C(51)-N(5)-Os(1)	126.3(4)
C(55)-N(5)-Os(1)	116.2(3)
O(1)-C(11)-C(12)	117.6(5)
O(1)-C(11)-C(16)	125.1(5)
C(12)-C(11)-C(16)	117.4(5)
C(13)-C(12)-C(11)	122.7(6)
C(13)-C(12)-H(12A)	118.7
C(11)-C(12)-H(12A)	118.7
C(12)-C(13)-C(14)	120.5(6)
C(12)-C(13)-H(13A)	119.7
C(14)-C(13)-H(13A)	119.7
C(15)-C(14)-C(13)	118.6(5)
C(15)-C(14)-H(14A)	120.7
C(13)-C(14)-H(14A)	120.7
C(14)-C(15)-C(16)	122.4(5)
C(14)-C(15)-H(15A)	118.8
C(16)-C(15)-H(15A)	118.8
C(15)-C(16)-C(11)	118.4(5)
C(15)-C(16)-C(61)	119.0(5)
C(11)-C(16)-C(61)	122.5(5)
N(2)-C(21)-C(22)	122.2(6)
N(2)-C(21)-H(21A)	118.9
C(22)-C(21)-H(21A)	118.9
C(21)-C(22)-C(23)	119.7(6)
C(21)-C(22)-H(22A)	120.2
C(23)-C(22)-H(22A)	120.2
C(24)-C(23)-C(22)	118.9(5)
C(24)-C(23)-H(23A)	120.5
C(22)-C(23)-H(23A)	120.5
C(23)-C(24)-C(25)	120.1(5)
C(23)-C(24)-H(24A)	120.0

C(25)-C(24)-H(24A)	120.0
N(2)-C(25)-C(24)	121.7(5)
N(2)-C(25)-C(35)	114.6(5)
C(24)-C(25)-C(35)	123.6(5)
N(3)-C(31)-C(32)	122.1(5)
N(3)-C(31)-H(31A)	118.9
C(32)-C(31)-H(31A)	118.9
C(31)-C(32)-C(33)	119.3(5)
C(31)-C(32)-H(32A)	120.4
C(33)-C(32)-H(32A)	120.4
C(34)-C(33)-C(32)	118.5(5)
C(34)-C(33)-H(33A)	120.7
C(32)-C(33)-H(33A)	120.7
C(33)-C(34)-C(35)	120.7(5)
C(33)-C(34)-H(34A)	119.7
C(35)-C(34)-H(34A)	119.7
C(34)-C(35)-N(3)	120.9(5)
C(34)-C(35)-C(25)	125.5(5)
N(3)-C(35)-C(25)	113.5(5)
N(4)-C(41)-C(42)	121.9(6)
N(4)-C(41)-H(41A)	119.0
C(42)-C(41)-H(41A)	119.0
C(43)-C(42)-C(41)	119.2(6)
C(43)-C(42)-H(42A)	120.4
C(41)-C(42)-H(42A)	120.4
C(42)-C(43)-C(44)	119.3(6)
C(42)-C(43)-H(43A)	120.3
C(44)-C(43)-H(43A)	120.3
C(45)-C(44)-C(43)	119.6(6)
C(45)-C(44)-H(44A)	120.2
C(43)-C(44)-H(44A)	120.2
N(4)-C(45)-C(44)	121.5(5)
N(4)-C(45)-C(55)	114.6(5)
C(44)-C(45)-C(55)	123.9(5)
N(5)-C(51)-C(52)	123.3(5)
N(5)-C(51)-H(51A)	118.4
C(52)-C(51)-H(51A)	118.4
C(51)-C(52)-C(53)	119.9(5)
C(51)-C(52)-H(52A)	120.1

C(53)-C(52)-H(52A)	120.1
C(54)-C(53)-C(52)	118.8(5)
C(54)-C(53)-H(53A)	120.6
C(52)-C(53)-H(53A)	120.6
C(53)-C(54)-C(55)	119.7(5)
C(53)-C(54)-H(54A)	120.2
C(55)-C(54)-H(54A)	120.2
N(5)-C(55)-C(54)	121.3(5)
N(5)-C(55)-C(45)	114.0(5)
C(54)-C(55)-C(45)	124.7(5)
N(1)-C(61)-O(2)	115.7(5)
N(1)-C(61)-C(16)	129.1(5)
O(2)-C(61)-C(16)	115.3(5)
O(2)-C(62)-C(67)	104.4(5)
O(2)-C(62)-C(66)	108.4(5)
C(67)-C(62)-C(66)	113.0(5)
O(2)-C(62)-C(63)	102.0(4)
C(67)-C(62)-C(63)	116.1(5)
C(66)-C(62)-C(63)	111.8(5)
N(1)-C(63)-C(64)	112.0(4)
N(1)-C(63)-C(62)	103.6(4)
C(64)-C(63)-C(62)	114.5(5)
N(1)-C(63)-H(63A)	108.8
C(64)-C(63)-H(63A)	108.8
C(62)-C(63)-H(63A)	108.8
C(63)-C(64)-S(1)	113.3(4)
C(63)-C(64)-H(64A)	108.9
S(1)-C(64)-H(64A)	108.9
C(63)-C(64)-H(64B)	108.9
S(1)-C(64)-H(64B)	108.9
H(64A)-C(64)-H(64B)	107.7
S(1)-C(65)-H(65A)	109.5
S(1)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5
S(1)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5
C(62)-C(66)-H(66A)	109.5
C(62)-C(66)-H(66B)	109.5

H(66A)-C(66)-H(66B)	109.5
C(62)-C(66)-H(66C)	109.5
H(66A)-C(66)-H(66C)	109.5
H(66B)-C(66)-H(66C)	109.5
C(62)-C(67)-H(67A)	109.5
C(62)-C(67)-H(67B)	109.5
H(67A)-C(67)-H(67B)	109.5
C(62)-C(67)-H(67C)	109.5
H(67A)-C(67)-H(67C)	109.5
H(67B)-C(67)-H(67C)	109.5
C(116)-C(111)-C(112)	114.7(5)
C(116)-C(111)-B(1)	124.5(5)
C(112)-C(111)-B(1)	120.7(5)
C(113)-C(112)-C(111)	123.4(6)
C(113)-C(112)-H(11A)	118.3
C(111)-C(112)-H(11A)	118.3
C(114)-C(113)-C(112)	120.3(6)
C(114)-C(113)-H(11B)	119.9
C(112)-C(113)-H(11B)	119.9
C(113)-C(114)-C(115)	119.5(6)
C(113)-C(114)-H(11C)	120.2
C(115)-C(114)-H(11C)	120.2
C(114)-C(115)-C(116)	119.6(6)
C(114)-C(115)-H(11D)	120.2
C(116)-C(115)-H(11D)	120.2
C(111)-C(116)-C(115)	122.6(6)
C(111)-C(116)-H(11E)	118.7
C(115)-C(116)-H(11E)	118.7
C(122)-C(121)-C(126)	115.6(5)
C(122)-C(121)-B(1)	125.1(5)
C(126)-C(121)-B(1)	119.3(6)
C(121)-C(122)-C(123)	122.2(6)
C(121)-C(122)-H(12B)	118.9
C(123)-C(122)-H(12B)	118.9
C(124)-C(123)-C(122)	119.6(7)
C(124)-C(123)-H(12C)	120.2
C(122)-C(123)-H(12C)	120.2
C(125)-C(124)-C(123)	119.9(6)
C(125)-C(124)-H(12D)	120.1

C(123)-C(124)-H(12D)	120.1
C(124)-C(125)-C(126)	119.5(6)
C(124)-C(125)-H(12E)	120.3
C(126)-C(125)-H(12E)	120.3
C(125)-C(126)-C(121)	123.2(6)
C(125)-C(126)-H(12F)	118.4
C(121)-C(126)-H(12F)	118.4
C(136)-C(131)-C(132)	116.4(5)
C(136)-C(131)-B(1)	123.9(5)
C(132)-C(131)-B(1)	119.6(5)
C(131)-C(132)-C(133)	122.2(6)
C(131)-C(132)-H(13B)	118.9
C(133)-C(132)-H(13B)	118.9
C(134)-C(133)-C(132)	120.0(6)
C(134)-C(133)-H(13C)	120.0
C(132)-C(133)-H(13C)	120.0
C(135)-C(134)-C(133)	118.8(6)
C(135)-C(134)-H(13D)	120.6
C(133)-C(134)-H(13D)	120.6
C(134)-C(135)-C(136)	120.6(6)
C(134)-C(135)-H(13E)	119.7
C(136)-C(135)-H(13E)	119.7
C(131)-C(136)-C(135)	122.0(6)
C(131)-C(136)-H(13F)	119.0
C(135)-C(136)-H(13F)	119.0
C(146)-C(141)-C(142)	115.0(6)
C(146)-C(141)-B(1)	125.8(5)
C(142)-C(141)-B(1)	119.2(5)
C(143)-C(142)-C(141)	122.9(6)
C(143)-C(142)-H(14B)	118.5
C(141)-C(142)-H(14B)	118.5
C(142)-C(143)-C(144)	121.1(6)
C(142)-C(143)-H(14C)	119.5
C(144)-C(143)-H(14C)	119.5
C(145)-C(144)-C(143)	117.3(6)
C(145)-C(144)-H(14D)	121.3
C(143)-C(144)-H(14D)	121.3
C(144)-C(145)-C(146)	121.4(6)
C(144)-C(145)-H(14E)	119.3

C(146)-C(145)-H(14E)	119.3
C(141)-C(146)-C(145)	122.3(6)
C(141)-C(146)-H(14F)	118.8
C(145)-C(146)-H(14F)	118.8
C(111)-B(1)-C(121)	113.0(5)
C(111)-B(1)-C(141)	110.1(5)
C(121)-B(1)-C(141)	107.0(5)
C(111)-B(1)-C(131)	105.1(5)
C(121)-B(1)-C(131)	109.5(5)
C(141)-B(1)-C(131)	112.2(5)

Table S10. Anisotropic displacement parameters ($Å^2$x 10^3) for Δ-**5** (BPh_4). The anisotropic displacement factor exponent takes the form: $-2^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Os(1)	20(1)	19(1)	16(1)	0(1)	-1(1)	0(1)
S(1)	31(1)	43(1)	32(1)	-7(1)	8(1)	8(1)
O(1)	16(2)	32(2)	20(2)	2(2)	2(2)	7(2)
O(2)	28(2)	35(2)	23(2)	9(2)	6(2)	0(2)
N(1)	22(3)	22(2)	11(2)	4(2)	3(2)	0(2)
N(2)	17(3)	27(2)	14(2)	1(2)	-3(2)	3(2)
N(3)	21(2)	18(2)	17(2)	-5(2)	-3(2)	-8(2)
N(4)	24(2)	23(2)	13(2)	9(2)	6(2)	2(2)
N(5)	13(2)	14(2)	22(2)	-2(2)	-4(2)	0(2)
C(11)	23(3)	25(3)	17(3)	-2(2)	-2(2)	3(2)
C(12)	27(3)	36(4)	23(3)	4(3)	5(3)	2(3)
C(13)	24(3)	41(4)	38(4)	0(3)	0(3)	12(3)
C(14)	36(4)	35(4)	27(3)	4(3)	-6(3)	12(3)
C(15)	31(4)	26(3)	20(3)	6(2)	5(3)	1(3)
C(16)	22(3)	21(3)	19(3)	2(2)	0(2)	0(2)
C(21)	36(3)	24(3)	21(3)	-3(2)	1(3)	1(3)
C(22)	31(4)	28(3)	24(3)	0(3)	4(3)	3(3)
C(23)	28(3)	40(4)	32(3)	1(3)	-5(2)	11(3)
C(24)	30(3)	30(3)	22(3)	-5(3)	-5(2)	-4(3)
C(25)	24(3)	26(3)	11(2)	0(2)	1(2)	3(2)
C(31)	36(4)	15(3)	26(3)	0(2)	3(2)	2(2)
C(32)	45(4)	19(3)	27(3)	0(3)	0(3)	4(3)
C(33)	38(4)	25(3)	24(3)	0(2)	3(3)	-7(3)
C(34)	25(3)	21(3)	23(3)	2(2)	-3(2)	-3(2)
C(35)	24(3)	21(3)	16(2)	-4(2)	2(2)	-2(3)
C(41)	40(4)	32(3)	17(3)	0(3)	-6(2)	-1(3)
C(42)	60(5)	43(4)	15(3)	2(3)	-2(3)	-6(3)
C(43)	68(5)	53(5)	20(3)	11(3)	-1(3)	-15(4)
C(44)	52(4)	29(4)	29(3)	5(3)	3(3)	-7(3)
C(45)	25(3)	26(3)	19(3)	2(2)	2(2)	-1(2)
C(51)	24(3)	21(3)	24(3)	-3(2)	1(2)	-4(2)
C(52)	24(3)	32(3)	24(3)	-7(3)	-4(3)	3(3)
C(53)	29(3)	28(3)	35(3)	-4(2)	5(3)	-5(3)

C(54)	27(4)	28(3)	36(4)	3(2)	10(3)	-6(3)
C(55)	20(3)	27(3)	23(3)	-1(2)	9(2)	4(2)
C(61)	28(3)	20(3)	15(3)	-2(2)	2(2)	-2(2)
C(62)	22(3)	41(4)	21(3)	4(3)	2(2)	1(3)
C(63)	23(3)	32(3)	14(3)	-1(2)	3(2)	0(2)
C(64)	24(3)	30(3)	23(3)	-4(2)	4(2)	-4(3)
C(65)	32(4)	80(6)	55(4)	-16(4)	7(4)	9(4)
C(66)	32(4)	48(4)	45(4)	17(3)	9(3)	0(3)
C(67)	55(4)	60(5)	20(3)	-7(3)	-8(3)	13(3)
C(111)	26(3)	23(3)	18(3)	-9(2)	4(3)	3(2)
C(112)	29(3)	31(3)	31(4)	-5(3)	6(3)	-2(3)
C(113)	33(4)	44(4)	38(4)	-12(3)	-8(3)	15(3)
C(114)	56(5)	31(4)	19(3)	-4(3)	-9(3)	19(3)
C(115)	47(4)	28(3)	21(3)	3(3)	7(3)	5(3)
C(116)	33(3)	25(3)	30(3)	-4(3)	-1(3)	5(3)
C(121)	26(3)	30(3)	26(3)	1(3)	6(3)	4(3)
C(122)	37(3)	34(3)	39(3)	3(3)	-4(4)	0(3)
C(123)	46(4)	32(4)	71(5)	-7(4)	-10(4)	-3(3)
C(124)	48(5)	23(3)	80(6)	-1(4)	5(4)	3(3)
C(125)	47(4)	35(4)	49(4)	14(4)	10(3)	12(4)
C(126)	40(3)	30(3)	31(3)	5(3)	5(3)	4(3)
C(131)	16(3)	32(3)	23(3)	4(2)	-7(3)	1(3)
C(132)	41(4)	28(3)	31(3)	2(2)	7(3)	-5(3)
C(133)	43(4)	38(4)	44(4)	-12(3)	0(3)	10(3)
C(134)	28(4)	51(4)	35(4)	-8(3)	2(3)	7(3)
C(135)	23(3)	47(4)	23(3)	1(3)	-2(2)	-2(3)
C(136)	18(3)	36(3)	25(3)	-4(3)	-5(2)	-1(3)
C(141)	33(3)	25(3)	23(3)	8(2)	2(3)	2(3)
C(142)	33(4)	29(3)	34(3)	-2(3)	1(3)	7(3)
C(143)	27(3)	35(3)	42(4)	4(3)	8(3)	1(3)
C(144)	26(3)	38(4)	40(4)	11(3)	-2(3)	-3(3)
C(145)	36(4)	44(4)	23(3)	7(3)	-7(3)	-10(3)
C(146)	34(4)	44(4)	20(3)	5(3)	3(3)	-4(3)
B(1)	31(4)	29(4)	20(3)	4(3)	-1(3)	-2(3)

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for Δ-**5** (BPh_4).

	x	y	z	U(eq)
H(12A)	-2929	6387	1065	34
H(13A)	-4019	7072	464	41
H(14A)	-2918	7316	-344	39
H(15A)	-691	6871	-512	31
H(21A)	3088	3975	1167	32
H(22A)	5240	3638	1513	33
H(23A)	6850	4469	1809	40
H(24A)	6195	5617	1794	33
H(31A)	795	6902	1188	31
H(32A)	2071	7883	1391	36
H(33A)	4479	7784	1637	34
H(34A)	5468	6696	1705	28
H(41A)	1596	5741	2246	36
H(42A)	813	5315	3048	47
H(43A)	-458	4296	3072	57
H(44A)	-960	3724	2290	44
H(51A)	427	4453	114	27
H(52A)	-957	3513	-38	32
H(53A)	-1899	2892	666	36
H(54A)	-1533	3294	1514	36
H(63A)	3868	5783	199	27
H(64A)	2726	4567	-275	31
H(64B)	3416	4570	297	31
H(65A)	7297	4804	94	83
H(65B)	6100	4553	495	83
H(65C)	6135	5337	303	83
H(66A)	3766	6690	-965	63
H(66B)	4886	6231	-649	63
H(66C)	3974	6801	-348	63
H(67A)	2355	5775	-1301	67
H(67B)	1640	5216	-924	67
H(67C)	3296	5171	-1055	67
H(11A)	1869	1721	1150	36

H(11B)	939	2380	487	46
H(11C)	2365	3145	28	43
H(11D)	4753	3245	246	38
H(11E)	5705	2564	916	35
H(12B)	3226	749	846	44
H(12C)	2932	-441	791	59
H(12D)	3761	-1146	1463	61
H(12E)	4966	-664	2168	52
H(12F)	5311	507	2203	41
H(13B)	4100	2869	2076	40
H(13C)	2712	3289	2758	50
H(13D)	1274	2540	3239	46
H(13E)	1215	1379	3013	38
H(13F)	2588	967	2327	32
H(14B)	6796	1290	1019	38
H(14C)	9196	1437	1097	42
H(14D)	10171	1962	1843	42
H(14E)	8633	2333	2496	41
H(14F)	6194	2228	2400	39

Table S12. Torsion angles [°] for Δ-**5** (BPh_4).

N(3)-Os(1)-O(1)-C(11)	77.2(4)
N(2)-Os(1)-O(1)-C(11)	126.9(9)
N(5)-Os(1)-O(1)-C(11)	-105.3(4)
N(4)-Os(1)-O(1)-C(11)	175.9(5)
N(1)-Os(1)-O(1)-C(11)	-8.8(4)
N(3)-Os(1)-N(1)-C(61)	-83.5(4)
N(2)-Os(1)-N(1)-C(61)	-161.2(4)
N(5)-Os(1)-N(1)-C(61)	95.5(4)
N(4)-Os(1)-N(1)-C(61)	56.0(17)
O(1)-Os(1)-N(1)-C(61)	11.2(4)
N(3)-Os(1)-N(1)-C(63)	82.5(4)
N(2)-Os(1)-N(1)-C(63)	4.7(4)
N(5)-Os(1)-N(1)-C(63)	-98.6(4)
N(4)-Os(1)-N(1)-C(63)	-138.1(14)
O(1)-Os(1)-N(1)-C(63)	177.1(4)
N(3)-Os(1)-N(2)-C(21)	172.3(5)
N(5)-Os(1)-N(2)-C(21)	-5.0(5)
N(4)-Os(1)-N(2)-C(21)	72.5(5)
O(1)-Os(1)-N(2)-C(21)	121.5(8)
N(1)-Os(1)-N(2)-C(21)	-103.5(4)
N(3)-Os(1)-N(2)-C(25)	3.5(4)
N(5)-Os(1)-N(2)-C(25)	-173.8(4)
N(4)-Os(1)-N(2)-C(25)	-96.4(4)
O(1)-Os(1)-N(2)-C(25)	-47.3(11)
N(1)-Os(1)-N(2)-C(25)	87.6(4)
N(2)-Os(1)-N(3)-C(31)	179.1(5)
N(5)-Os(1)-N(3)-C(31)	-79(4)
N(4)-Os(1)-N(3)-C(31)	-96.8(4)
O(1)-Os(1)-N(3)-C(31)	-9.3(4)
N(1)-Os(1)-N(3)-C(31)	78.8(4)
N(2)-Os(1)-N(3)-C(35)	0.3(4)
N(5)-Os(1)-N(3)-C(35)	102(4)
N(4)-Os(1)-N(3)-C(35)	84.4(4)
O(1)-Os(1)-N(3)-C(35)	171.8(4)
N(1)-Os(1)-N(3)-C(35)	-100.0(4)
N(3)-Os(1)-N(4)-C(41)	-1.6(5)
N(2)-Os(1)-N(4)-C(41)	76.2(5)

N(5)-Os(1)-N(4)-C(41)	179.3(5)
O(1)-Os(1)-N(4)-C(41)	-95.6(4)
N(1)-Os(1)-N(4)-C(41)	-140.5(14)
N(3)-Os(1)-N(4)-C(45)	178.6(4)
N(2)-Os(1)-N(4)-C(45)	-103.6(4)
N(5)-Os(1)-N(4)-C(45)	-0.5(4)
O(1)-Os(1)-N(4)-C(45)	84.6(4)
N(1)-Os(1)-N(4)-C(45)	39.7(17)
N(3)-Os(1)-N(5)-C(51)	157(4)
N(2)-Os(1)-N(5)-C(51)	-101.6(4)
N(4)-Os(1)-N(5)-C(51)	175.0(5)
O(1)-Os(1)-N(5)-C(51)	87.2(4)
N(1)-Os(1)-N(5)-C(51)	-0.6(4)
N(3)-Os(1)-N(5)-C(55)	-15(4)
N(2)-Os(1)-N(5)-C(55)	85.9(4)
N(4)-Os(1)-N(5)-C(55)	2.5(4)
O(1)-Os(1)-N(5)-C(55)	-85.4(4)
N(1)-Os(1)-N(5)-C(55)	-173.2(4)
Os(1)-O(1)-C(11)-C(12)	-173.3(4)
Os(1)-O(1)-C(11)-C(16)	4.6(8)
O(1)-C(11)-C(12)-C(13)	-179.8(6)
C(16)-C(11)-C(12)-C(13)	2.1(9)
C(11)-C(12)-C(13)-C(14)	-0.6(10)
C(12)-C(13)-C(14)-C(15)	-0.9(10)
C(13)-C(14)-C(15)-C(16)	0.8(9)
C(14)-C(15)-C(16)-C(11)	0.8(8)
C(14)-C(15)-C(16)-C(61)	179.6(5)
O(1)-C(11)-C(16)-C(15)	179.8(5)
C(12)-C(11)-C(16)-C(15)	-2.2(8)
O(1)-C(11)-C(16)-C(61)	1.1(9)
C(12)-C(11)-C(16)-C(61)	179.1(5)
C(25)-N(2)-C(21)-C(22)	-1.1(8)
Os(1)-N(2)-C(21)-C(22)	-169.9(4)
N(2)-C(21)-C(22)-C(23)	-0.4(9)
C(21)-C(22)-C(23)-C(24)	1.9(8)
C(22)-C(23)-C(24)-C(25)	-2.0(8)
C(21)-N(2)-C(25)-C(24)	1.1(8)
Os(1)-N(2)-C(25)-C(24)	170.9(4)
C(21)-N(2)-C(25)-C(35)	-176.2(5)

Os(1)-N(2)-C(25)-C(35)	-6.4(6)
C(23)-C(24)-C(25)-N(2)	0.4(8)
C(23)-C(24)-C(25)-C(35)	177.5(5)
C(35)-N(3)-C(31)-C(32)	2.0(8)
Os(1)-N(3)-C(31)-C(32)	-176.8(4)
N(3)-C(31)-C(32)-C(33)	-1.4(9)
C(31)-C(32)-C(33)-C(34)	-1.4(8)
C(32)-C(33)-C(34)-C(35)	3.6(8)
C(33)-C(34)-C(35)-N(3)	-3.1(8)
C(33)-C(34)-C(35)-C(25)	180.0(5)
C(31)-N(3)-C(35)-C(34)	0.2(7)
Os(1)-N(3)-C(35)-C(34)	179.1(4)
C(31)-N(3)-C(35)-C(25)	177.5(5)
Os(1)-N(3)-C(35)-C(25)	-3.6(6)
N(2)-C(25)-C(35)-C(34)	-176.4(5)
C(24)-C(25)-C(35)-C(34)	6.3(8)
N(2)-C(25)-C(35)-N(3)	6.4(6)
C(24)-C(25)-C(35)-N(3)	-170.8(5)
C(45)-N(4)-C(41)-C(42)	-1.0(8)
Os(1)-N(4)-C(41)-C(42)	179.3(5)
N(4)-C(41)-C(42)-C(43)	1.0(10)
C(41)-C(42)-C(43)-C(44)	-0.4(11)
C(42)-C(43)-C(44)-C(45)	-0.2(11)
C(41)-N(4)-C(45)-C(44)	0.3(8)
Os(1)-N(4)-C(45)-C(44)	-179.9(5)
C(41)-N(4)-C(45)-C(55)	178.8(5)
Os(1)-N(4)-C(45)-C(55)	-1.4(6)
C(43)-C(44)-C(45)-N(4)	0.3(10)
C(43)-C(44)-C(45)-C(55)	-178.1(6)
C(55)-N(5)-C(51)-C(52)	-1.0(8)
Os(1)-N(5)-C(51)-C(52)	-173.5(4)
N(5)-C(51)-C(52)-C(53)	-0.7(9)
C(51)-C(52)-C(53)-C(54)	2.3(9)
C(52)-C(53)-C(54)-C(55)	-2.1(10)
C(51)-N(5)-C(55)-C(54)	1.1(8)
Os(1)-N(5)-C(55)-C(54)	174.4(4)
C(51)-N(5)-C(55)-C(45)	-177.1(5)
Os(1)-N(5)-C(55)-C(45)	-3.9(6)
C(53)-C(54)-C(55)-N(5)	0.4(9)

C(53)-C(54)-C(55)-C(45)	178.5(6)
N(4)-C(45)-C(55)-N(5)	3.4(7)
C(44)-C(45)-C(55)-N(5)	-178.1(6)
N(4)-C(45)-C(55)-C(54)	-174.8(5)
C(44)-C(45)-C(55)-C(54)	3.7(9)
C(63)-N(1)-C(61)-O(2)	1.2(6)
Os(1)-N(1)-C(61)-O(2)	169.2(3)
C(63)-N(1)-C(61)-C(16)	-178.5(5)
Os(1)-N(1)-C(61)-C(16)	-10.5(8)
C(62)-O(2)-C(61)-N(1)	5.7(6)
C(62)-O(2)-C(61)-C(16)	-174.6(4)
C(15)-C(16)-C(61)-N(1)	-176.2(5)
C(11)-C(16)-C(61)-N(1)	2.5(9)
C(15)-C(16)-C(61)-O(2)	4.1(7)
C(11)-C(16)-C(61)-O(2)	-177.2(5)
C(61)-O(2)-C(62)-C(67)	112.0(5)
C(61)-O(2)-C(62)-C(66)	-127.4(5)
C(61)-O(2)-C(62)-C(63)	-9.3(5)
C(61)-N(1)-C(63)-C(64)	-131.0(5)
Os(1)-N(1)-C(63)-C(64)	61.3(6)
C(61)-N(1)-C(63)-C(62)	-7.0(6)
Os(1)-N(1)-C(63)-C(62)	-174.8(3)
O(2)-C(62)-C(63)-N(1)	9.6(5)
C(67)-C(62)-C(63)-N(1)	-103.3(6)
C(66)-C(62)-C(63)-N(1)	125.1(5)
O(2)-C(62)-C(63)-C(64)	131.9(5)
C(67)-C(62)-C(63)-C(64)	19.1(7)
C(66)-C(62)-C(63)-C(64)	-112.5(6)
N(1)-C(63)-C(64)-S(1)	-173.0(3)
C(62)-C(63)-C(64)-S(1)	69.3(6)
C(65)-S(1)-C(64)-C(63)	74.4(5)
C(116)-C(111)-C(112)-C(113)	0.5(8)
B(1)-C(111)-C(112)-C(113)	176.2(5)
C(111)-C(112)-C(113)-C(114)	-0.4(9)
C(112)-C(113)-C(114)-C(115)	-0.2(9)
C(113)-C(114)-C(115)-C(116)	0.5(9)
C(112)-C(111)-C(116)-C(115)	-0.1(8)
B(1)-C(111)-C(116)-C(115)	-175.6(5)
C(114)-C(115)-C(116)-C(111)	-0.4(9)

C(126)-C(121)-C(122)-C(123)	1.1(9)
B(1)-C(121)-C(122)-C(123)	-177.5(6)
C(121)-C(122)-C(123)-C(124)	0.8(10)
C(122)-C(123)-C(124)-C(125)	-1.6(11)
C(123)-C(124)-C(125)-C(126)	0.5(10)
C(124)-C(125)-C(126)-C(121)	1.5(10)
C(122)-C(121)-C(126)-C(125)	-2.2(9)
B(1)-C(121)-C(126)-C(125)	176.4(6)
C(136)-C(131)-C(132)-C(133)	0.5(9)
B(1)-C(131)-C(132)-C(133)	177.5(6)
C(131)-C(132)-C(133)-C(134)	0.3(10)
C(132)-C(133)-C(134)-C(135)	-0.8(10)
C(133)-C(134)-C(135)-C(136)	0.5(9)
C(132)-C(131)-C(136)-C(135)	-0.8(8)
B(1)-C(131)-C(136)-C(135)	-177.6(5)
C(134)-C(135)-C(136)-C(131)	0.3(9)
C(146)-C(141)-C(142)-C(143)	-0.3(8)
B(1)-C(141)-C(142)-C(143)	-178.9(5)
C(141)-C(142)-C(143)-C(144)	1.0(9)
C(142)-C(143)-C(144)-C(145)	-0.3(9)
C(143)-C(144)-C(145)-C(146)	-1.2(9)
C(142)-C(141)-C(146)-C(145)	-1.2(9)
B(1)-C(141)-C(146)-C(145)	177.3(6)
C(144)-C(145)-C(146)-C(141)	2.0(10)
C(116)-C(111)-B(1)-C(121)	-123.7(6)
C(112)-C(111)-B(1)-C(121)	61.1(7)
C(116)-C(111)-B(1)-C(141)	-4.1(7)
C(112)-C(111)-B(1)-C(141)	-179.3(5)
C(116)-C(111)-B(1)-C(131)	116.9(6)
C(112)-C(111)-B(1)-C(131)	-58.3(6)
C(122)-C(121)-B(1)-C(111)	-5.4(9)
C(126)-C(121)-B(1)-C(111)	176.1(5)
C(122)-C(121)-B(1)-C(141)	-126.7(6)
C(126)-C(121)-B(1)-C(141)	54.7(7)
C(122)-C(121)-B(1)-C(131)	111.4(6)
C(126)-C(121)-B(1)-C(131)	-67.1(7)
C(146)-C(141)-B(1)-C(111)	114.6(6)
C(142)-C(141)-B(1)-C(111)	-66.9(6)
C(146)-C(141)-B(1)-C(121)	-122.2(6)

C(142)-C(141)-B(1)-C(121)	56.3(6)
C(146)-C(141)-B(1)-C(131)	-2.1(8)
C(142)-C(141)-B(1)-C(131)	176.4(5)
C(136)-C(131)-B(1)-C(111)	118.8(6)
C(132)-C(131)-B(1)-C(111)	-57.9(7)
C(136)-C(131)-B(1)-C(121)	-2.9(8)
C(132)-C(131)-B(1)-C(121)	-179.5(5)
C(136)-C(131)-B(1)-C(141)	-121.5(6)
C(132)-C(131)-B(1)-C(141)	61.8(7)

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