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Supporting Information

Is the Hoveyda-Grubbs Complex a Vinylogous Fischer-type Carbene? Aromaticity-Controlled Activity of Ruthenium Metathesis Catalysts

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Contents

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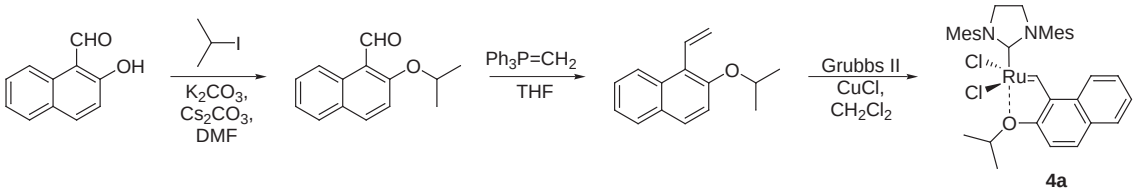
1. General

All reactions were carried out under argon in a pre-dried glassware using Schlenk techniques. Solvents were dried by distillation over the following agents and transferred under argon: THF (K/benzophenone), toluene (Na), *n*-pentane, *n*-hexane, CH_2Cl_2 and DMF (CaH_2), Et_2O ($LiAlH_4$), MeOH (Mg). Flash column chromatography was performed on silica gel 60 (230–400 mesh). NMR: Spectra were recorded in $CDCl_3$; chemical shifts (δ) are given in ppm relative to TMS, coupling constants (J) in Hz. IR: wavenumbers in cm^{-1}. MS (EI, LSIMS): AMD 604 Intectra GmbH. MS (ESI): Micromass LCT with Lock-Spray unit. Injections were made after dissolving the sample in MeCN. Molecular formulas of synthesized ruthenium compounds were confirmed by comparison of theoretical and experimental molecular isotope patterns. GC: HP 6890 with HP 5 column. GC/MS: HP 5890 with HP 5 column. Microanalyses were provided by the Institute of Organic Chemistry, PAS, Warsaw.

All commercially available chemicals were used as received.

2. Synthesis of complex 4a



2-Hydroxy-1-naphthaldehyde was obtained from Aldrich.

2.1. Alkylation of 2-hydroxy-1-naphthaldehyde

To a suspension of K_2CO_3 (2.6 g; 19.1 mmol) and Cs_2CO_3 (0.9 g; 2.7 mmol) in DMF (25 mL), 2-hydroxy-1-naphthaldehyde (2.2 g; 12.7 mmol) was added. After stirring for 30 min at RT, 2-jodopropane (1.9 mL; 3.2 g; 19.1 mmol) was added and the reaction mixture was stirred at RT overnight. Then mixture was poured into water (40 mL) and extracted with diethyl ether. The combined extracts were washed with brine, water and dried. The solvent was evaporated to obtain 2-isopropoxy-1-naphthaldehyde (2.4 g; 89%) as orange crystals. IR (film in DCM): ν 3062, 2982, 2936, 2876, 1689, 1682, 1625, 1599, 1510, 1468, 1450, 1402, 1387, 1374, 1338, 1215, 1187, 1181, 1156, 1137, 1113, 1101, 1012, 974, 950, 941, 942, 912, 868, 841, 814, 623, 505 cm^{-1}. ^{1}H NMR (200 MHz, $CDCl_3$) δ 1.52 (d, $J = 6.0$ Hz, 6H), 4.90 (septet, $J = 6.0$ Hz, 1H), 7.30-7.38 (m, 1H), 7.44-7.52 (m, 1H), 7.62-7.74 (m, 1H), 7.78-7.90 (m, 1H), 8.04-8.12 (m, 1H), 9.34-9.44 (m, 1H), 10.98 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 22.2, 72.5, 115.2, 118.0, 124.8, 128.1, 128.4, 129.6, 131.6, 137.2, 162.8, 192.4. MS (EI) *m/z* (rel intensity) 214 (77, $M^{+\cdot}$), 186 (18), 145 (11), 144 (100), 127 (4), 116 (14), 115 (38), 89 (6), 63 (5), 41 (5), 39 (5). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{14}H_{14}O_2$): 214.09938; found: 214.10023. Mp = 64-66 °C. Anal. Calcd. for $C_{14}H_{14}O_2$: C 78.48, H 6.59. Found C 78.26, H 6.43.

2.2. Wittig reaction of 2-isopropoxy-1-naphthaldehyde

In a three-necked flask solid methyltriphenylphosphonium bromide (5.5 g; 15.4 mmol; Aldrich) and THF (65 mL) were placed under argon. Then solution of n-BuLi (7.6 mL; 15.4 mmol) was added dropwise at 78 °C. After 30 min solution of 2-isopropoxy-1-naphthaldehyde (2.4 g; 11 mmol) in THF (16 mL) was

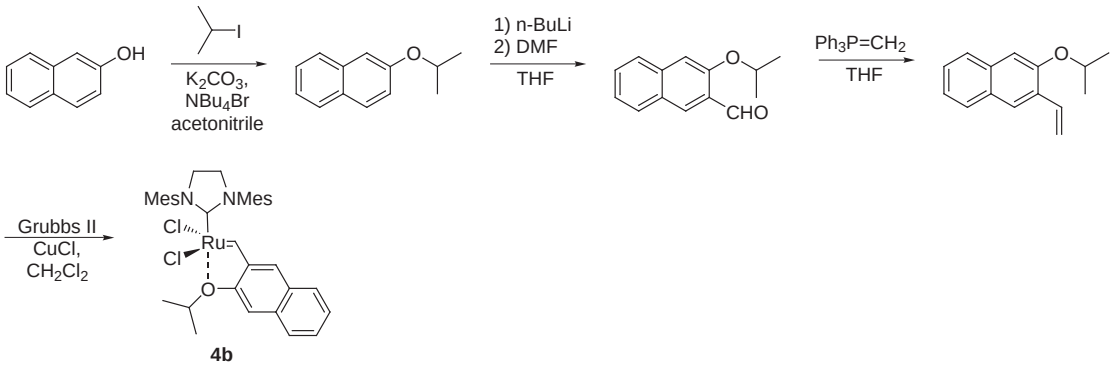
added and the reaction mixture was stirred for 1h. After warming to RT mixture was stirred for 18h, treated with saturated solution of NH_4Cl, extracted with *tert*-butyl methyl ether and dried over $MgSO_4$. The solvent was evaporated and the product was purified by short column chromatography (*c*-hexane ethyl acetate 2:8) to obtain 2-isopropoxy-1-vinylnaphthalene (1.3 g; 56%) as a yellow oil. IR (film in DCM): ν 3684, 2980, 2933, 2874, 1842, 1678, 1628, 1591, 1508, 1464, 1432, 1419, 1383, 1372, 1331, 1302, 1242, 1172, 1137, 1113, 1044, 1023, 991, 927, 903, 864, 826, 809, 603, 548, 520 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$) δ 1.36 (d, J = 6.1 Hz, 6H), 4.59-4.69 (m, 1H), 5.71 (dd, J = 11.5, 2.2 Hz, 1H), 5.76 (dd, J = 18.0, 2.4 Hz, 1H), 7.10 (dd, J = 18.0, 6.2 Hz, 1H), 7.22-7.25 (m, 1H), 7.32-7.36 (m, 1H), 7.42-7.48 (m, 1H), 7.68-7.78 (m, 2H), 8.16-8.24 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.5, 72.1, 117.0, 120.5, 123.2, 123.6, 124.4, 126.2, 128.2, 128.5, 129.4, 130.6, 132.5, 152.8. MS (EI) *m/z* (rel intensity) 212 (34, $M^{+\cdot}$), 171 (14), 170 (100), 169 (92), 153 (17), 141 (36), 139 (18), 115 (34), 43 (10), 41 (11). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{15}H_{16}O$): 212.12012; found: 212.11932. Anal. Calcd. for $C_{15}H_{16}O$: C 84.87, H 7.60. Found C 84.73, H 7.51.

2.3. Ligand exchange reaction

2-Isopropoxy-1-vinylnaphthalene (0.051 g; 0.24 mmol), CuCl (0.024 g; 0.24 mmol) and CH_2Cl_2 (15 mL) were placed in a Schlenk flask. Afterwards Grubbs second generation carbene complex (0.17 g; 0.20 mmol) was added and the resulted solution was stirred under argon at 40 °C for 30 min. From this point forth all manipulations were carried out in air with reagent-grade solvents. The reaction mixture was concentrated under vacuum and the resulted material was dissolved in ethyl acetate (ca. 10 mL), white solid was filtered off and the filtrate was concentrated under vacuum. The product was purified by column chromatography. Elution with *c*-hexane, then *c*-hexane ethyl actate (1 : 1) removed **4a** as a light green band. Solvent was evaporated and product dissolved in small amount of CH_2Cl_2, then methanol was added until green crystals precipitated. The precipitate was filtered off, washed with methanol and dried *in vacuo* to afford complex **4a** (0.030 g, 22%) as a light green solid. IR (KBr): ν 3436, 3052, 3022, 2959, 2917, 2737, 1944, 1619, 1607, 1581, 1566, 1512, 1481, 1449, 1432, 1420, 1397, 1383, 1346, 1316, 1294, 1259, 1218, 1196, 1078, 1049, 1038, 1003, 1034, 985, 967, 916, 896, 878, 852, 813, 753, 695, 645, 616, 579, 557, 527, 512, 475, 437, 420 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$) δ 1.25-1.40 (m, 6H), 2.20-2.80 (m, 18H), 4.16 (s, 4H), 5.03-5.15 (m, 1H), 7.00-7.20 (m, 5H), 7.22-7.30 (m, 1H) 7.32-7.40 (m, 2H), 7.45-7.56 (m, 1H), 7.70-7.76 (m, 1H), 8.10-8.18 (m, 1H), 18.15 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 21.1, 21.3, 52.2, 114.4, 123.6, 124.3, 124.7, 126.4, 126.5, 127.0, 127.6, 128.7, 129.4, 129.6, 130.2, 130.7, 137.3, 138.8, 138.9, 150.3, 211.9, 290.5. MS (EI) *m/z* (rel intensity) 677 (13), 676 (6, $M^{+\cdot}$) 598 (12), 562 (14), 559 (29), 404 (22), 403 (6), 399 (18), 311 (9), 310 (19), 305 (39), 304 (22), 303 (22), 281 (14), 280 (12), 199 (17), 198 (44), 169 (13), 158 (34), 157 (17), 129 (13), 117 (100), 116 (24), 115 (25), 83 (22), 81 (17), 78 (10), 55 (31), 43 (14), 41 (30). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{35}H_{40}N_2O_1{}^{35}Cl_2{}^{102}Ru$): 676.15612; found: 676.15027. Anal. Calcd. for $C_{35}H_{40}N_2OCl_2Ru$: C 62.12, H 6.40, N 4.04, Cl 10.24. Found C 62.30, H 6.35, N 4.27, Cl 10.51.

The green solid was dissolved in small amount CH_2Cl_2, some amount of methanol was added and left in open flask overnight at RT.

3. Synthesis of complex 4b



2-Naphthol was available from Aldrich.

3.1. Alkylation of 2-naphthol

2-Naphthol (14.417 g; 0.1 mol), 2-iodopropane (34.147 g; 0.2 mol), tetrabutylammonium hydrogen sulphate (0.681 g; 0.002 mol), K_2CO_3 (55.182 g; 0.4 mol) and acetonitrile (100 mL) were stirred vigorously at 45 °C 24 h. Then mixture was filtered, residue was washed with acetonitrile and combined organic solution were concentrated *in vacuo*. Then ethyl acetate (200 mL) and water (200 mL) were added, organic phase was washed with 1 M aqueous solution of NaOH (4×50 mL), brine (2×50 mL) and dried $MgSO_4$. Solution was filtered, concentrated *in vacuo* and distilled to obtain: 14.45 g (0.0776 mol; 78 %) of red oil. IR (film in DCM): ν 3580, 2981, 2936, 2876, 1948, 1904, 1832, 1628, 1600, 1581, 1510, 1468, 1440, 1388, 1373, 1356, 1334, 1216, 1188, 1171, 1137, 1118, 1019, 974, 941, 900, 871, 842, 814, 675, 645, 623, 532 cm^{-1}. ^1H NMR (200 MHz, $CDCl_3$) δ 1.45 (d, J = 6.0 Hz, 6H), 4.66-4.82 (m, 1H), 7.13-7.18 (m, 2H), 7.28-7.48 (m, 2H), 7.68-7.82 (m, 3H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 22.0, 69.8, 108.4, 119.7, 123.4, 126.2, 126.6, 127.6, 128.8, 129.3, 134.6, 155.7. MS (EI) *m/z* (rel intensity) 186 (18, $M^{+\cdot}$), 145 (11), 144 (100), 127 (4), 116 (11), 115 (34), 89 (5), 63 (4), 43 (3), 41 (4), 39 (4). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{13}H_{14}O$): 186.10447; found: 186.10497.

3.2. Formylation of 2-isopropoxynaphthalene

To the solution of 2-isopropoxynaphthalene (1.841 g; 10 mmol) in THF (18 mL) at RT under argon, solution of *n*-BuLi (4.2 mL, 11.34 mmol, 2.7 M in heptane) was added slowly. Mixture was stirred for 2.5 h, cooled to -78 °C and solution of DMF (2.848 g; 39 mmol) in THF (4 mL) was added slowly. After 10 minutes cooling bath was removed, flask was warmed to 0 °C and quenched with aqueous solution of NH_4Cl. Then diluted solution of HCl was added and mixture was stirred overnight. Next water (100 mL) was added and mixture was extracted with ethyl acetate, combined organic phases were washed with brine and dried with $MgSO_4$. After chromatographic separation (hexanes - ethyl acetate mixture) yellowish oil (2-isopropoxy-3-naphthaldehyde) was obtained (0.325 g; 1.52 mmol; 15%)[2] IR (film in DCM): ν 3685, 3253, 3061, 2982, 2935, 2860, 1688, 1625, 1598, 1545, 1503, 1450, 1438, 1403, 1386, 1375, 1356, 1336, 1253, 1186, 1157, 1137, 1117, 1101, 1064, 1026, 951, 921, 920, 892, 868, 834, 787, 622, 605, 542, 504 cm^{-1}. ^1H NMR (200 MHz, $CDCl_3$) δ 1.40-1.52 (m, 6H), 4.74-4.88 (m, 1H), 7.16-7.22 (m, 1H), 7.36-7.40 (m, 1H), 7.52-7.58 (m, 2H), 7.69-7.75 (m, 1H), 7.85-7.90 (m, 1H), 8.35-8.39 (m, 1H), 10.61 (s, 1H). ^{13}C NMR (50 MHz, $CDCl_3$) δ 21.9,70.8, 108.4, 124.4, 126.3, 126.5, 127.5, 129.0, 129.9, 130.3, 137.6, 156.0, 190.6. MS

[2] Unidentified compound (probably product of formylation in position 1) was also observed.

(EI) *m/z* (rel intensity) 214 (15, $M^{+\cdot}$), 173 (12), 172 (100), 171 (48), 126 (12), 116 (13), 115 (48), 114 (9), 89 (8), 41 (8). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{14}H_{14}O_2$): 214.09938; found: 214.09913. Anal. Calcd. for $C_{14}H_{14}O_2$: C 78.48, H 6.59. Found C 78.31, H 6.74.

3.3. Wittig reaction of 2-isopropoxy-3-naphthaldehyde

In three-necked flask solid methyltriphenylphosphonium bromide (1.0 g; 2.8 mmol, Aldrich) and THF (10 mL) were placed under argon. Then a solution of n-BuLi (1.8 mL; 2.8 mmol; 1.6 M) was added dropwise at 78 °C. After 30 min a solution of 2-isopropoxy-3-naphthaldehyde (0.3 g; 1.4 mmol) in THF (2 mL) was added and the reaction mixture was stirred for 1h. After warming to RT reaction mixture was stirred for 18h, treated with saturated aqueous solution of NH_4Cl, extracted with *tetr*buthyl methyl ether and dried over $MgSO_4$. Solvent was evaporated and product was purified by short column chromatography (*c*-hexane ethyl acetate 2:8) to obtain 2-isopropoxy-3-vinylnaphthalene (0.19 g; 64%) as a yellow oil. IR (film in DCM): ν 3686, 3601, 3087, 3024, 2981, 2936, 2875, 2639, 2366, 1947, 1841, 1691, 1629, 1599, 1498, 1465, 1450, 1416, 1386, 1374, 1361, 1333, 1298, 1226, 1189, 1169, 1150, 1136, 1115, 1044, 1018, 997, 949, 916, 896, 865, 835, 807, 659, 622, 529 cm^{-1}. ^1H NMR (400 MHz, CDCl) δ 1.391.46 (m, 6H), 4.70 (septet, J = 6.1 Hz, 1H), 5.34 (d, J = 11.2, 1.7 Hz, 1H), 5.90 (d, J = 17.6, 1.7 Hz, 1H), 7.08-7.24 (m, 2H), 7.26-7.32 (m, 1H), 7.35-7.42 (m, 1H), 7.60-7.80 (m, 2H), 7.90 (s, 1H). ^{13}C NMR (100 MHz, CDCl) δ 22.0, 70.3, 107.7, 115.3, 123.7, 125.9, 126.1, 126.2, 127.7, 128.5, 129.3, 132.4, 134.1, 153.7. MS (EI) *m/z* (rel intensity) 213 (6), 212 (39, $M^{+\cdot}$), 171 (13), 170 (100), 142 (34), 141 (49), 139 (13), 115 (25), 43 (9) 41 (8). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{15}H_{16}O$): 212.09938; found: 212.9913. Anal. Calcd. for $C_{15}H_{16}O$: C 84.87, H 7.60. Found C 84.65, H 7.43.

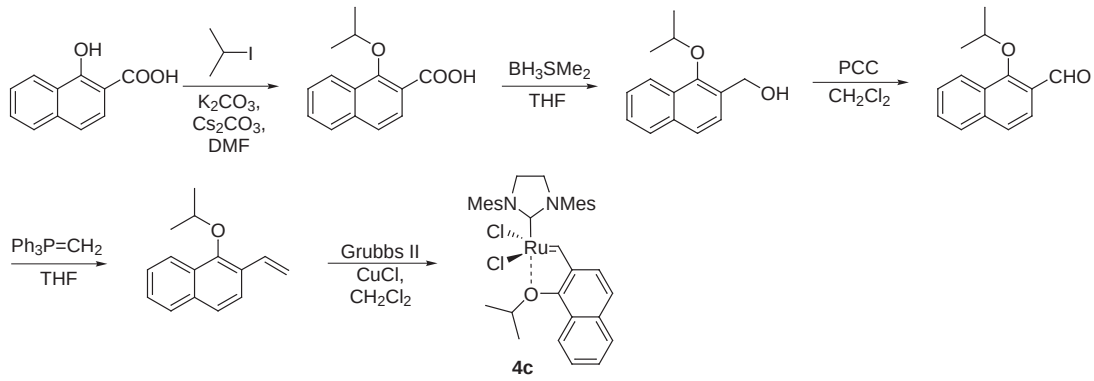
3.4. Ligand exchange reaction

2-Isopropoxy-3-vinylnaphthalene (0.0187 g; 0.088 mmol), CuCl (0.01 g; 0.088 mmol) and CH_2Cl_2 (4.5 mL) were placed in a Schlenk flask. Afterwards Grubbs second generation carbene complex (0.068 g; 0.08 mmol) was added and the resulted solution was stirred under argon at 40 °C for 20 min. From this point forth all manipulations were carried out in air with reagent-grade solvents. The reaction mixture was concentrated *in vacuo* and the residue was dissolved in ethyl acetate (ca. 3 mL), white solid was filtered off and the filtrate was concentrated under vacuum. The product was purified by column chromatography. Elution with *c*-hexane (ca. 100 mL), then *c*-hexane ethyl acetate (1:1) removed complex **4b** as a green band. The solvent was evaporated and product dissolved in a small amount ethyl acetate, then *n*-pentane was added until green crystals precipitated. The precipitate was filtered off, washed with *n*-pentane and dried *in vacuo* to afford complex **4b** (0.043 g; 78%) as a green solid. IR (KBr): ν 3445, 2968, 2912, 2735, 1618, 1598, 1571, 1503, 1481, 1447, 1419, 1397, 1382, 1336, 1317, 1295, 1261, 1182, 1137, 1106, 1034, 991, 935, 913, 894, 859, 851, 783, 745, 698, 645, 623, 579, 534, 474, 443, 420 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$) δ 1.32 (d, J = 6.1 Hz, 6H), 2.35-2.55 (m, 18H), 4.17 (s, 4H), 4.94-5.02 (m, 1H), 6.98 (s, 1H), 7.09 (s, 4H), 7.22-7.28 (m, 1H), 7.56 (s, 1H), 7.50-7.58 (m, 2H), 7.86-7.92 (m, 1H), 16.75 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 19.2, 19.5, 21.0, 21.1, 51.5, 108.3, 120.6, 125.4, 127.0, 127.7, 129.4, 130.1, 133.8, 138.8, 139.1, 146.2, 150.2, 211.0, 296.3. MS (EI) *m/z* (rel intensity) 681 (12), 680 (35), 679 (35), 678 (88), 677 (53), 676 (94, $M^{+\cdot}$), 675 (56), 674 (37), 673 (23), 672 (11), 670 (11), 598 (12), 565 (17), 564 (49), 563 (38), 562 (100), 561 (69), 559 (55), 558 (28), 557 (21), 556 (20), 534 (13), 533 (12), 532 (11), 531 (10), 442 (10), 441 (11), 440 (10), 408 (11), 407 (19), 406 (25), 405 (40), 404 (37), 403 (33), 402 (32), 401 (25), 400 (26), 399 (21), 398 (17), 397 (14), 396 (10), 394 (14), 392 (22), 391 (16), 390 (19), 389 (16), 388 (15), 387 (11), 386

(14), 308 (11), 307 (48), 306 (14), 305 (49), 304 (51), 303 (39), 301 (29), 289 (11), 287 (25), 159 (10), 158 (33), 146 (13), 145 (10), 144 (11), 128 (12), 99 (11). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{35}H_{40}N_2O^{35}Cl_2{}^{102}Ru$): 676.15612; found: 676.15027 Anal. Calcd. for $C_{35}H_{40}N_2O^{35}Cl_2{}^{102}Ru$: C 62.12, H 5.96, N 4.14, Cl 10.48. Found C 62.24, H 6.03, N 4.30, Cl 10.55.

The green solid was dissolved in small amount of ethyl acetate and *n*-pentane and left in open flask overnight at RT.

4. Synthesis of complex 4c



1-Hydroxy-2-naphthoic acid was available fom Aldrich.

4.1. Alkylation of 1-hydroxy-2-naphthoic acid

To a suspension of K_2CO_3(9.4 g; 68 mmol) and Cs_2CO_3 (1.7 g; 5 mmol) in DMF (30 ml), 1-hydroxy-2-naphthoic acid (3.2 g; 17 mmol) was added. After stirring for 30 min, 2-jodopropane(5 mL, 8.7 g, 51 mmol) was added and reaction mixture was stirred overnight at RT. Then mixture was poured into water (50 mL) and extracted with diethyl ether. The combined extracts were washed with water, brine and dried. The solvent was evaporated and 1-isopropoxy-2-naphthoic acid (3.2 g; 69%) was obtained as a light pink crystals. IR (film in DCM): ν 3197, 2983, 2937, 2686, 2522, 2411, 2306, 1739, 1626, 1599, 1570, 1506, 1460, 1432, 1378, 1189, 1141, 1123, 1098, 1065, 1025, 918, 901, 892, 872, 839, 811, 622, 601, 569 cm^{-1}. ^1H NMR (400 MHz, CDCl) δ 1.47 (d, J = 6.2 Hz, 6H), 4.77 (septet, J = 6.2 Hz, 1H), 7.55-7.66 (m, 2H), 7.67-7.74 (m, 1H), 7.86-7.93 (m, 1H), 8.09-8.13 (m, 2H), 11.56 (s, 1H). ^{13}C NMR (100 MHz, CDCl) δ 22.0, 80.9, 119.3, 123.2, 124.8, 126.6, 126.8, 127.3, 128.5, 128.8, 137.5, 154.4, 166.5. MS (EI) *m/z* (rel intensity) 230 (6, $M^{+\cdot}$), 189 (3), 188 (21), 171 (15), 170 (100), 142 (7), 115 (7), 114 (24), 113 (3). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{14}H_{14}O_3$): 230.09429; found: 230.09482. Anal. Calcd. for $C_{14}H_{14}O_3$: C 73.03, H 6.13. Found C 73.23, H 6.29. Mp = 73-75 °C.

4.2. Reduction of 1-isopropoxy-2-naphthoic acid

To a solution of 1-isopropoxy-2-naphthoic acid (0.42 g, 1.84 mmol) in THF (3 mL) at 5 °C under argon borane dimethyl sulfide complex (0.5 mL, 5.52 mmol) was added dropwise with vigorous stirring. After evolution of gas cooling bath was removed and mixture was left at RT for 24 h. Methanol (1

mL) was added slowly, mixture was evaporated *in vacuo* and diethyl ether (30 mL) was added. Solution was washed with saturated K_2CO_3 and brine. Combined aqueous phases were extracted with ethyl acetate, washed with brine, combined with etheral solution and dried with $MgSO_4$. Solvent was evaporated and the residue was purified by column chromatography (*c*-hexane ethyl acetate 2 : 5) to obtain 2-hydroxymethyl-1-isopropoxynaphthalene (0.27 g; 66 %) as an orange oil. IR (film in DCM): ν 3603, 2980, 2933, 2686, 2522, 2411, 2306, 1911, 1824, 1665, 1629, 1598, 1572, 1507, 1466, 1454, 1432, 1383, 1373, 1332, 1187, 1139, 1106, 1083, 1028, 969, 931, 901, 892, 870, 816, 784, 663, 612, 560 cm^{-1}. ^{1}H NMR (400 MHz, CDCl) δ 1.37 (d, J = 6.2 Hz, 6H), 4.46 (septet, 1H)6.2, 4.90 (s, 1H), 7.40-7.52 (m, 3H), 7.57-7.63 (m, 1H), 7.72-7.85 (m, 1H), 8.05-8.15 (m, 1H). ^{13}C NMR (100 MHz, CDCl) δ 22.6, 61.4, 122.8. 124.0, 125.7, 126.0, 126.5, 128.0, 128.8, 129.6, 134.6, 151.2. MS (EI) *m/z* (rel intensity) 217 (2), 216 (14, $M^{+\cdot}$), 174 (11), 172 (2), 171 (3), 158 (2), 157 (13), 156 (100), 145 (2), 129 (5), 128 (34), 127 (11), 126 (3), 115 (7), 77 (3). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{14}H_{16}O_2$): 216.11503; found: 216.11422. Anal. Calcd. for $C_{14}H_{16}O_2$: C 77.75, H 7.46. Found C 77.59, H 7.63.

4.3. Oxidation of 2-hydroxymethyl-1-isopropoxynaphthalene

2-Hydroxymethyl-1-isopropoxynaphthalene was dissolved in CH_2Cl_2 (12 mL), PCC (0.4 g; 1.9 mmol) was added slowly and mixture was stirred at RT for 1 h. The liquid was separated on column chromatography with (*c*-hexane ethyl acetate 5:1) to give 1-isopropoxy-2-naphthaldehyde (0.23 g; 86%) as an yellow oil. IR (film in DCM): ν 3335, 3060, 2976, 2930, 2870, 2735, 1924, 1674, 1623, 1597, 1573, 1506, 1459, 1432, 1383, 1373, 1335, 1262, 1229, 1189, 1142, 1101, 1082, 1025, 934, 911, 871, 816, 785, 769, 750, 730, 723, 675, 634, 599, 567, 515, 493, 473, 433 cm^{-1}. ^{1}H NMR (400 MHz, CDCl) δ 1.43 (d, J = 6.1 Hz, 6H), 4.52 (septet, J = 6.1 Hz, 1H), 7.53-7.59 (m, 1H), 7.60-7.65 (m, 2H), 7.84-7.90 (m, 2H), 8.20-8.24 (m, 1H), 10.57 (s, 1H). ^{13}C NMR (100 MHz, CDCl) δ 22.4, 80.6, 122.6, 124.0, 124.2, 126.1, 126.4, 128.3, 128.9, 129.2, 138.0, 160.2, 190.2. MS (EI) *m/z* (rel intensity) 214 (5, $M^{+\cdot}$), 173 (12), 172 (100), 171 (65), 170 (7), 154 (5), 144 (4), 143 (8), 126 (8), 116 (4), 115 (27), 114 (5). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{14}H_{14}O_2$): 214.09938; found: 214.09854. Anal. Calcd. for $C_{14}H_{14}O_2$: C 78.48, H 6.95. Found C 78.55, H 6.71.

4.4. Wittig reaction of 1-isopropoxy-2-naphthaldehyde

In Schlenk flask solid methyltriphenylphosphonium bromide (0.39 g; 1.1 mmol, Aldrich) and toluene (8 mL) were placed under argon. Then a solution of potassium *tert*-pentylate (0.64 mL; 1.1 mmol; 1.7 M in toluene, Fluka) was added dropwise at 5 °C. Reaction mixture was warmed to RT and stirred for 2 h. Then mixture was cooled to 5 °C and a solution of 1-isopropoxy-2-naphthaldehyde (0.19 g; 0.87 mmol) in toluene (4 mL) was added, mixture was allowed to warm up to RT and was stirred overnight. Then saturated solution of NH_4Cl was added, mixture was extracted with *tert*-butyl methyl ether and dried over $MgSO_4$. Solvent was evaporated and product was purified by short column chromatography (*c*-hexane ethyl acetate 2 : 3) to obtain 1-isopropoxy-2-vinylnaphthalene (0.134 g; 73%) as an yellow oil. IR (film in DCM): ν 2979, 2928, 2855, 1912, 1829, 1721, 1672, 1627, 1564, 1506, 1465, 1454, 1433, 1418, 1379, 1332, 1298, 1241, 1188, 1139, 1106, 1081, 1027, 1003, 962, 933, 912, 870, 816, 788, 643, 620, 575, 558 cm^{-1}. ^{1}H NMR (400 MHz, CDCl) δ 1.36 (d, J = 6.2 Hz, 6H), 4.41 (m, J = 6.2 Hz, 1H), 5.35 (dd, J = 11.0, 1.3 Hz, 1H), 5.81 (dd, J = 16.7, 1.1 Hz, 1H), 7.20-7.25 (m, 1H), 7.40-7.50 (m, 2H), 7.53-7.58 (m, 1H), 7.64-7.69 (m, 1H), 7.75-7.81 (m, 1H), 8.11-8.16 (m, 1H). ^{13}C NMR (100 MHz, CDCl) δ 22.6, 114.0, 123.3, 123.6, 125.7, 126.0, 126.7, 127.7, 129.5, 132.3, 134.5, 151.2. MS (EI) *m/z* (rel intensity) 212 (19, $M^{+\cdot}$), 171 (14), 170 (100), 169 (33), 168 (5), 142 (15), 141 (58), 140 (6), 139 (17), 115 (33). HRMS (EI) calcd for $M^{+\cdot}$

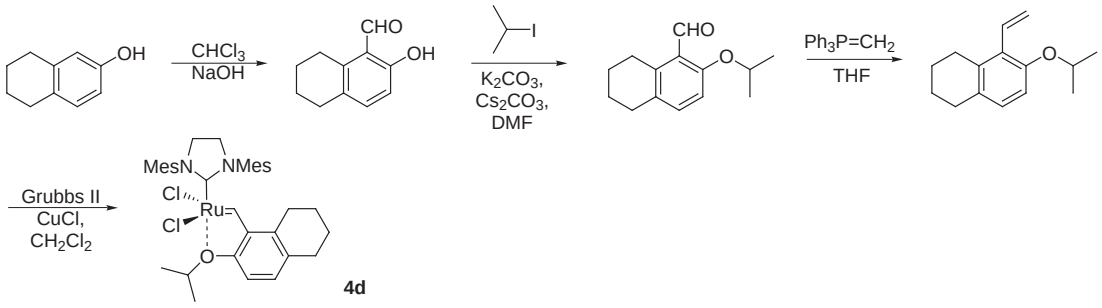
($C_{15}H_{16}O$): 212.12012; found: 212.12076. Anal. Calcd. for $C_{15}H_{16}O$: C 84.87, H 7.60. Found C 84.79, H 7.86.

4.5. Ligand exchange reaction

1-Isopropoxy-2-vinylnaphthalene (0.035 g; 0.17 mmol), CuCl (0.0163 g; 0.17 mmol) and CH_2Cl_2 (7.5 mL) were placed in a Schlenk flask. Afterwards Grubbs second generation carbene complex (0.127 g; 0.15 mmol) was added and the resulted solution was stirred under argon at 40 °C for 30 min. From this point forth all manipulations were carried out in air with reagent-grade solvents. The reaction mixture was concentrated under vacuum and the resulted material was dissolved in ethyl acetate (ca. 15 mL), white solid was filtered off and the filtrate was concentrated under vacuum. The product was purified by column chromatography. Elution with *c*-hexane (ca. 150 mL), then *c*-hexane ethyl acetate (3 : 1) removed **4c** as a green band. The solvent was evaporated and product dissolved in small amount CH_2Cl_2, then *n*-pentan was added until green crystals precipitated. The precipitate was filtered off, washed with *n*-pentane and dried *in vacuo* to afford complex **4c** (0.03 g, 30%) as a green solid. IR (KBr): ν 3377, 3019, 2921, 2857, 1941, 1700, 1653, 1617, 1607, 1581, 1566, 1512, 1480, 1448, 1442, 1420, 1397, 1380, 1348, 1315, 1293, 1258, 1220, 1196, 1149, 1137, 1100, 1034, 984, 943, 919, 895, 878, 853, 814, 753, 695, 667, 644, 616, 578, 557, 513, 482, 437 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$) δ 1.32-1.39 (m, 6H), 2.20-2.80 (m, 18H), 4.18 (s, 4H), 5.05-5.15 (m, 1H), 7.09-7.11 (m, 4H), 7.23-7.32 (m, 1H), 7.33-7.39 (m, 1H), 7.45-7.55 (m, 1H), 7.70-7.80 (m, 1H), 8.14-8.15 (m, 1H), 18.19 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 21.1, 21.3, 114.4, 123.6, 124.3, 124.6, 126.4, 126.5, 127.0, 127.6, 128.6, 128.7, 130.2, 130.7, 138.8, 138.9, 150.3, 211.9, 290.5. MS (EI) *m/z* (rel intensity) 677 (3), 676 (16, $M^{+\cdot}$) 597 (7), 560 (5), 557 (15), 405 (6), 401 (8), 314 (11), 310 (14), 305 (22), 304 (83), 303 (74), 289 (19), 170 (16), 169 (18), 159 (18), 158 (88), 157 (34), 144 (13), 141 (12), 130 (13), 129 (35), 128 (28), 127 (12), 115 (20), 78 (15), 77 (10), 63 (22), 43 (100), 42 (15), 41 (43), 39 (26), 36 (16). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{35}H_{40}N_2O^{35}Cl_2{}^{102}Ru$): 676.15612; found: 676.15343. Anal. Calcd. for $C_{35}H_{40}N_2OCl_2Ru$: C 62.12, H 5.96, N 4.14, Cl 10.48. Found C 62.39, H 6.11, N 4.27, Cl 10.61.

Attempts of crystallization were unsuccessful.

5. Synthesis of complex 4d



1,2,3,4-tetrahydro-6-naphthol was available from Aldrich.

6-hydroxy-1,2,3,4-tetrahydro-5-naphthaldehyde was prepared from 1,2,3,4-tetrahydro-6-naphthol in Riermer-Tiemann rection according to the procedure described in literature.[3]

[3] R. T. Arnold, H. E. Zaugg, J. Sprung, *J. Am. Chem. Soc.* **1941**, *63*, 1314-1316.

5.1. Alkylation of 6-hydroxy-1,2,3,4-tetrahydro-5-naphthaldehyde

To a suspension of K_2CO_3 (0.3 g; 2.1 mmol) and Cs_2CO_3 (0.0582 g; 0.2 mmol) in DMF (5 ml), 6-hydroxy-1,2,3,4-tetrahydro-5-naphthaldehyde (0.15 g; 0.9 mmol) was added under argon. After stirring for 30 min at RT, 2-jodopropane (0.13 mL, 0.22 g, 1.3 mmol) was added and the reaction mixture was stirred for 2 h at RT. Then mixture was poured into water (10 mL) and extracted with diethyl ether. The combined extracts were washed with brine, water and dried. The solvent was evaporated to obtain 2-isopropoxy-5,6,7,8-tetrahydronaphthalene-1-carbaldehyde (0.12 g; 65 %) as a yellow oil. IR (film in DCM): ν 3534, 3031, 2977, 2932, 2860, 2838, 2778, 1681, 1609, 1592, 1580, 1488, 1474, 1423, 1408, 1384, 1373, 1354, 1324, 1274, 1250, 1220, 1203, 1182, 1167, 1136, 1113, 1077, 1054, 1013, 992, 969, 937, 905, 889, 865, 828, 807, 733, 679, 613, 469 cm^{-1}. ^{1}H NMR (400 MHz, CDCl) δ 1.36 (m, J = 6.1 Hz, 6H), 1.68-1.82 (m, 4H), 2.67-2.75 (m, 2H), 3.05-3.11 (m, 2H), 4.60 (septet, J = 6.1 Hz, 1H), 6.76-6.82 (m, 1H), 7.18-7.22 (m, 1H), 10.64 (s, 1H). ^{13}C NMR (100 MHz, CDCl) δ 22.1, 22.4, 22.9, 27.9, 29.5, 71.4, 111.7, 123.8, 130.0, 135.7, 140.7, 160.3, 193.4.. MS (EI) *m/z* (rel intensity) 218 (32, $M^{+\cdot}$), 177 (12), 176 (100), 175 (31), 161 (8), 158 (6), 148 (43), 147 (71), 115 (6) 91 (11) 41 (8). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{14}H_{18}O_2$): 218.13068; found: 218.12965. Anal. Calcd. for $C_{14}H_{18}O_2$: C 77.03, H 8.31. Found C 77.24, H 8.52.

5.2. Wittig reaction of 2-isopropoxy-5,6,7,8-tetrahydronaphthalene-1-carbaldehyde

In a Schlenk flask solid methyltriphenylphosphonium bromide (0.22 g; 0.6 mmol, Aldrich) and toluene (4 mL) were placed under argon. Then a solution of potassium *tert*-pentylate (0.36 mL; 0.6 mmol; 1.7 M in toluene, Fluka) was added dropwise at 5 °C . After warming to RT mixture was stirred for 2 h, then cooled to 5 °Cand a solution of 2-isopropoxy-5,6,7,8-tetrahydronaphthalene-1-carbaldehyde (0.1 g; 0.5 mmol) in toluene (2 mL) was added. Mixture was allowed to warm to RT and stirred overnight. Then saturated solution of NH_4Cl was added, mixture was extracted with *tert*-butyl methyl ether and dried over $MgSO_4$. The solvent was evaporated and product was purified by short column chromatography (*c*-hexane ethyl acetate 2 : 3) to obtain 2-isopropoxy-3-vinyl-5,6,7,8-tetrahydronaphthalene (0.08 g; 78 %) as an yellow oil. IR (film in DCM): ν 3086, 3013, 2976, 2930, 2858, 2839, 2661, 2513, 1987, 1833, 1626, 1581, 1497, 1473, 1451, 1438, 1382, 1371, 1356, 1336, 1309, 1256, 1221, 1167, 1135, 1117, 1070, 1040, 1023, 982, 967, 915, 881, 849, 831, 798, 762, 733, 696, 655, 625, 578, 542, 468, 437 cm^{-1}. ^{1}H NMR (400 MHz, CDCl) δ 1.31 (d, J = 6.1 Hz, 6H), 1.70-1.80 (m, 4H), 2.68-2.78 (m, 2H), 4.42-4.52 (septet, J = 6.1 Hz, 1H), 5.48 (dd, J = 11.7, 2.4 Hz, 1H), 5.64 (dd, J = 18.0, 2.4 Hz, 1H), 6.64-6.76 (m, 2H), 6.80-7.04 (m, 1H). ^{13}C NMR (100 MHz, CDCl) δ 22.3, 22.9, 23.5, 26.9, 28.1, 29.5, 70.8, 112.2, 119.3, 127.0, 128.5, 129.6, 131.2, 136.3, 153.7. MS (EI) *m/z* (rel intensity) 216 (41, $M^{+\cdot}$), 174 (100), 173 (23), 160 (10), 159 (80), 147 (10), 146 (45), 145 (51), 144 (10), 131 (32), 129 (11), 128 (16), 127 (10), 117 (14), 115 (25), 91 (14). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{15}H_{20}O$): 216.15093; found: 216.15142. Anal. Calcd. for $C_{15}H_{20}O$: C 83.29, H 9.32. Found C 83.48, H 9.54.

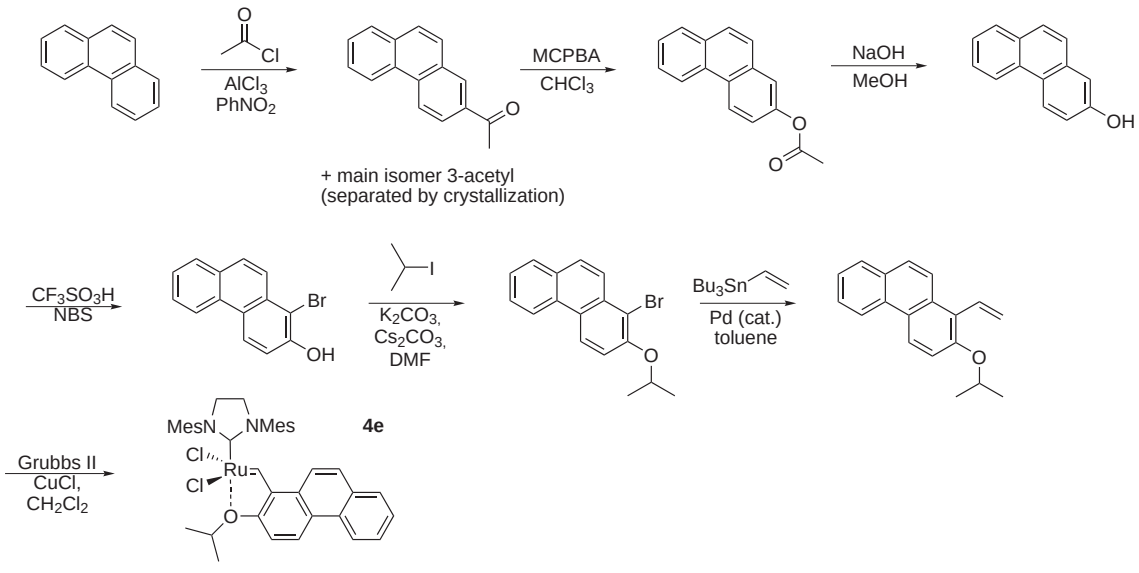
5.3. Ligand exchange reaction

2-Isopropoxy-3-vinyl-5,6,7,8-tetrahydronaphthalene (0.024 g; 0.11 mmol), CuCl (0.011 g; 0.11 mmol) and CH_2Cl_2 (4.5 mL) were placed in a Schlenk tube. Then Grubbs catalyst (0.085 g; 0.1 mmol) was added and the resulted solution was stirred under argon at 40 °C for 20 min. From this point forth all manipulations were carried out in air with reagent-grade solvents. The reaction mixture was concentrated under vacuum and the resulted material was dissolved in ethyl acetate (ca. 6 mL), white solid was filtered off and the filtrate was concentrated under vacuum. The product was purified by column chromatography.

Elution with c-hexane (ca. 150 ml), then c-hexane ethyl acetate (2:8) removed **4d** as a green band. The solvent was evaporated and the product was obtained as a green microcrystalline solid (0.023 g, 27%). IR (KBr): ν 3444, 2923, 2737, 2224, 1954, 1954, 1737, 1597, 1483, 1447, 1419, 1396, 1383, 1355, 1315, 1295, 1259, 1215, 1166, 1158, 1138, 1103, 1036, 967, 925, 919, 883, 851, 817, 802, 732, 702, 645, 604, 591, 579, 547, 473, 457, 441, 419 cm^{-1}. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.23-36 (m, 6H), 1.70-1.74 (m, 4H), 2.40-2.47 (m, 4H), 2.65-2.80 (m, 18H), 4.13 (s, 4H), 4.42-4.50 (m, 1H), 6.46 (s, 1H), 6.65-6.75 (m, 3H), 6.80-7.50 (m, 2H), 16.39 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 21.0, 21.1, 22.2, 22.3, 22.7, 22.9, 23.3, 23.5, 28.1, 29.4, 29.5, 30.7, 112.3, 113.7, 119.3, 126.5, 127.1, 127.6, 128.2, 128.6, 129.6, 131.2, 136.3, 137.3, 139.7, 150.3, 153.7, 212.6, 297.7. MS (EI) *m/z* (rel intensity) 684 (14), 683 (14), 682 (32), 681 (21), 680 (35, $M^{+\cdot}$), 679 (23), 678 (15), 604 (11), 602 (17), 601 (11), 568 (20), 567 (18), 566 (40), 565 (33), 564 (31), 563 (27), 562 (17), 561 (13), 560 (12), 442 (13), 440 (11), 408 (21), 407 (19), 406 (51), 405 (37), 404 (47), 403 (39), 402 (30), 401 (25), 400 (31), 399 (23), 398 (21), 397 (15), 396 (11), 395 (11), 307 (29), 306 (20), 305 (82), 304 (100), 303 (74), 302 (16), 301 (41), 290 (15), 298 (30), 288 (11), 287 (24), 273 (10), 216 (10), 204 (10), 174 (23), 162 (27), 161 (16), 160 (13), 159 (26), 158 (33), 148 (12), 147 (23), 146 (26), 145 (29), 144 (22), 134 (31), 131 (21), 130 (13), 129 (10), 128 (13), 119 (12), 117 (20), 116 (11), 115 (22), 105 (10), 103 (11), 91 (33), 77 (18). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{35}H_{44}N_2O^{35}Cl_2{}^{102}Ru$): 680.18742; found: 680.18608. Anal. Calcd. for $C_{35}H_{44}N_2OCl_2Ru$: C 61.76, H 6.52, N 4.12, Cl 10.42. Found C 61.63, H 6.49, N 4.33, Cl 10.68.

Crystals for X-Ray measurements were obtained by slow diffusion of n-pentane from solution of **4d** in ethyl acetate, in refrigerator.

6. Synthesis of complex 4e



Phenanthrene was available from Aldrich.

2-Acethylphenanthrene was prepared in Friedel-Crafts acylation reaction of phenanthrene described in literature.[4]

[4] E. Mosseting, J. van de Kamp, *J. Am. Chem. Soc.* **1930**, *52*, 3704-3710.

6.1. Baeyer-Villiger oxidation of 2-acetylphenanthrene

2-Acetylphenanthrene (0.5 g; 2.3 mmol) was dissolved in chloroform (30 mL) and *m*-CPBA (1.4 g; 9.2 mmol) was added slowly. Reaction mixture was refluxed overnight. Solution was washed with saturated K_2CO_3, water, brine and dried $MgSO_4$. Solvent was evaporated and the residue was purified by column chromatography (*c*-hexane ethyl acetate 3 : 1) to obtain 2-acetoxyphenanthrene (0.35 g; 66%) as a white solid. IR (film in DCM): ν 3578, 3405, 2987, 2929, 2855, 2686, 2523, 2126, 1926, 1733, 1684, 1622, 1605, 1575, 1531, 1499, 1465, 1439, 1422, 1408, 1361, 1312, 1233, 1208, 1177, 1145, 1096, 1038, 952, 896, 869, 859, 827, 809, 661, 625, 577, 554 cm^{-1}. ^1H NMR (400 MHz, CDCl) δ 2.37 (s, 3H), 7.37-7.39 (m, 1H), 7.40-7.42 (m, $J =$, Hz, 1H) 7.60-7.62 (m, 1H), 7.66-7.67 (m, 1H), 7.68 (s, 1H), 7.72-7.77 (m, 1H), 8.60-8.64 (m, 1H), 8.68-8.69 (m, 1H). ^{13}C NMR (100 MHz, CDCl) δ 21.2, 119.7, 120.8, 122.6, 124.2, 126.4, 126.5, 126.8, 127.9, 128.2, 128.6, 130.0, 131.8, 132.8, 149.0, 169.6. MS (EI) *m/z* (rel intensity) 236 (16, $M^{+\cdot}$), 220 (16), 205 (24), 195 (16), 194 (100), 177 (15), 176 (9), 166 (4), 165 (19) 163 (4) 88 (7). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{16}H_{12}O_2$): 236.08373; found: 236.08413. Anal. Calcd. for $C_{16}H_{12}O_2$: C 81.34, H 5.12. Found C 81.63, H 5.26. Mp = 112-114 °C.

6.2. Hydrolysis of 2-acetoxyphenanthrene

2-Acetoxyphenanthrene (0.16 g; 0.7 mmol) and NaOH (0.06 g; 1.4 mmol) were dissolved in methanol (15 mL) and heated under reflux for 1 h. Reaction mixture was acidified, extracted with diethyl ether combined organic phases were washed with brine and dried with $MgSO_4$. Solvent was evaporated and the residue was purified by column chromatography (*c*-hexane ethyl acetate 4 : 1) to obtain 2-phenanthrol (0.13 g; 95 %) as a white solid. IR (film in DCM): ν 2928, 2854, 2318, 2756, 1682, 1619, 1573, 1529, 1496, 1462, 1426, 1371, 1304, 1211, 1165, 1154, 1097, 1014, 1002, 959, 905, 874, 811, 651, 596 cm^{-1}. ^1H NMR (400 MHz, $(CD_3)_2CO$) δ 3.05 (s, 1H) 7.27-7.36 (m, 1H), 7.48-7.54 (m, 1H), 7.58-7.63 (m, 1H), 7.64-7.68 (m, 1H), 7.71-7.76 (m, 1H), 7.86-7.90 (m, 1H), 8.60-8.80 (m, 3H). ^{13}C NMR (100 MHz, CDCl) δ 112.3, 118.0, 122.8, 124.6, 125.2, 126.2, 127.0, 127.5, 128.0, 129.3, 131.5, 131.7, 134.7, 206.2. MS (EI) *m/z* (rel intensity) 195 (15) 194 (100, $M^{+\cdot}$), 166 (6), 165 (27), 164 (4), 163 (5), 97 (12), 83 (5), 82 (2), 82 (3). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{14}H_{10}O$): 194.07317; found: 194.07392. Anal. Calcd. for $C_{14}H_{10}O$: C 86.57, H 5.19. Found C 86.79, H 5.31. Mp = 105-107 °C.

6.3. Bromination of 2-phenanthrol

In a flask 2-phenanthrol (0.1 g, 0.52 mmol) was dissolved in acetonitrile (7 mL) and resulted solution was cooled to -17 °C. Trifluoromethanesulfonic acid(0.044 mL, 0.076 g, 0.57 mmol) was added slowly, followed by *N*-Bromosuccinimide. Reaction mixture was allowed to warm to RT and stirred overnight. Then solution of $Na_2S_2O_5$ in water (0.4 g/6 mL) was added, mixture was extracted with diethyl ether, washed with brine and dried over $MgSO_4$. Solvent was evaporated and product was purified by column chromatography (*c*-hexane ethyl acetate 5 : 1) to obtain 1-bromo-2-hydroxyphenanthrene (0.1 g; 71 %) as a white solid. IR (film in DCM): ν 3944, 3758, 3691, 3505, 2985, 2929, 2855, 2686, 2522, 2411, 2306, 2126, 2055, 1959, 1611, 1570, 1529, 1460, 1434, 1416, 1379, 1356, 1368, 1207, 1089, 1051, 1102, 1040, 1011, 981, 895, 867, 815, 794, 595, 533 cm^{-1}. ^1H NMR (400 MHz, CDCl) δ 5.95 (s, 1H), 7.33-7.43 (m, 1H), 7.50-7.60 (m, 1H), 7.60-7.70 (m, 1H), 7.78-7.86 (m, 1H), 7.86-7.93 (m, 1H), 7.98-8.08 (m, 1H), 8.52-8.62 (m, 2H). ^{13}C NMR (100 MHz, CDCl) δ 108.6, 116.1, 122.3, 123.7, 124.3, 125.8, 126.2, 127.2, 128.7, 129.2, 130.1, 130.7, 131.1, 151.2. MS (EI) *m/z* (rel intensity) 275 (14), 274 (100), 273 (16), 272 (79, $M^{+\cdot}$), 165 (59), 164 (68), 163 (76), 83 (12), 82 (10) 81 (13). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{14}H_9O^{79}Br$): 271.98368; found:

271.98282. Anal. Calcd. for $C_{14}H_9OBr$: C 61.57, H 3.32, Br 29.25. Found C 61.77, H 3.48, Br 29.37. Mp = 121-123 °C.

6.4. Alkylation of 1-bromo-2-hydroxyphenanthrene

To a suspension of K_2CO_3 (0.15 g; 1.1 mmol) and Cs_2CO_3 (0.023 g; 0.074 mmol) in DMF (8 ml), 1-bromo-2-hydroxyphenanthrene (0.096 g; 0.35 mmol) was added. After stirring for 30 min, 2-jodopropane (0.052 mL, 0.089 g, 0.53 mmol) was added and reaction mixture was stirred for 1 h at RT. Then mixture was poured into water (5 mL), extracted with diethyl ether, combined organic phases were washed with water, brine and dried. Solvent was evaporated to obtain 1-bromo-2-isopropoxyphenanthrene (0.09 g; 82%) as a white solid. IR (film in DCM): ν 3056, 2977, 2932, 1916, 1877, 1808, 1739, 1607, 1592, 1523, 1484, 1455, 1413, 1384, 1372, 1353, 1329, 1298, 1267, 1254, 1224, 1199, 1183, 1158, 1147, 1137, 1107, 1096, 1039, 1014, 960, 945, 906, 861, 833, 818, 809, 781, 784, 745, 711, 695, 640, 616, 557, 545, 523, 497, 466, 415 cm^{-1}. ^1H NMR (400 MHz, CDCl) δ 1.48 (d, J = 6.2 Hz, 6H), 4.73 (septet, J = 6.1 Hz, 1H), 7.28-7.36 (m, 1H), 7.53-7.60 (m, 1H), 7.61-7.68 (m, 1H), 7.78-7.83 (m, 1H), 7.86-7.90 (m, 1H), 8.20-8.27 (m, 1H), 8.55-8.63 (m, 1H). ^{13}C NMR (100 MHz, CDCl) δ 22.1, 22.4, 22.9, 27.9, 29.5, 71.4, 111.7, 123.8, 130.0, 135.7, 140.7, 160.3, 193.4. MS (EI) *m/z* (rel intensity) 316 (17) 314 (17, $M^{+\cdot}$), 275 (15), 274 (99), 273 (16), 272 (100), 245 (10), 243 (10), 165 (30), 164 (38), 163 (42). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{17}H_{15}O^{79}Br$): 314.03063; found: 314.02953. Anal. Calcd. for $C_{17}H_{15}OBr$: C 64.78, H 4.80, Br 25.35. Found C 64.57, H 4.89, Br 25.61. Mp = 125-126 °C

6.5. Stille reaction of 1-bromo-2-isopropoxyphenanthrene

In a Schlenk flask was placed $Pd(PPh_3)_4$ (0.015 g; 3 mol%) and a solution of 1-bromo-2-isopropoxyphenanthrene (0.134 g; 0.425 mmol) in toluene (2 mL) was added under argon. Neat $Bu_3SnCH{=}CH_2$ (0.15 g; 0.47 mmol) was added *via* syringe and resulting solution was heated at 120 °C for 4 hours. After cooling to RT solvent was evaporated and a solution of KF (0.50 g) in methanol (5 mL) was added to the residue. Mixture was stirred at RT for 2 h and evaporated. To the resulting residue *tert*-butyl methyl ether (15 mL) and water (10 mL) were added. Organic phase was removed, aqueous phase was extracted and combined organic phases were dried and evaporated. The product was purified by column chromatography (*c*-hexane ethyl acetate 5 : 1) to give 1-vinyl-2-isopropoxyphenanthrene (0.072 g; 65%) as an yellowish solid. IR (film in DCM): ν 3086, 3059, 342, 3018, 2975, 2932, 2870, 2494, 2017, 1934, 1907, 1880, 1827, 1801, 1732, 1687, 1622, 1606, 1584, 1574, 1525, 1490, 1459, 1420, 1406, 1382, 1373, 13336, 1297, 1265, 1250, 1199, 1073, 1057, 1034, 1110, 1047, 1032, 1007, 992, 939, 911, 869, 860, 825, 812, 769, 748, 699, 685, 647, 598, 570, 532, 510, 493, 466, 417 cm^{-1}. ^1H NMR (400 MHz, CDCl) δ 1.40 (d, J = 6.2 Hz, 6H), 4.69 (septet, 1H)6.2, 5.74 (td, J = 17.8, 2.2 Hz, 2H), 7.12 (dd, J = 17.8, 6.2 Hz, 1H), 7.30-7.35 (m, 1H), 7.50-7.55 (m, 1H), 7.58-7.64 (m, 1H), 7.67-7.72 (m, J = , Hz, 1H) 7.80-7.87 (m, 1H), 8.12-8.20 (m, 1H), 8.53-8.62 (m, 2H). ^{13}C NMR (100 MHz, CDCl) δ 22.4, 71.7, 115.2, 121.0, 122.3, 122.9, 123.7, 124.8, 125.0, 125.7, 126.6, 127.2, 128.3, 130.6, 130.7, 131.1, 131.2, 153.8. MS (EI) *m/z* (rel intensity) 262 (38, $M^{+\cdot}$), 221 (17), 220 (100), 219 (73), 218 (14), 203 (31), 202 (14), 191 (30), 190 (19), 189 (45), 165 (14). HRMS (EI) calcd for $M^{+\cdot}$ ($C_{19}H_{18}O$): 262.13577; found: 262.13615. Anal. Calcd. for $C_{19}H_{18}O$: C 86.99, H 6.92. Found C 86.75, H 6.85. Mp = 102-104 °C.

6.6. Ligand exchange procedure

1-Vinyl-2-isopropoxyphenanthrene (0.041 g; 0.15 mmol), CuCl (0.015 g; 0.15 mmol) and CH_2Cl_2 (7 mL) were placed in a Schlenk flask. Afterwards Grubbs second generation carbene complex (0.119 g; 0.14 mmol) was added and the resulted solution was stirred under argon at 40 °C for 30 min. From this point forth all manipulations were carried out in air with reagent-grade solvents. The reaction mixture was concentrated under vacuum and the resulted material was dissolved in ethyl acetate (ca. 15 mL), white solid was filtered off and the filtrate was concentrated under vacuum. The product was purified by column chromatography. Elution with *c*-hexane (ca. 150 mL), then *c*-hexane ethyl acetate (5 : 1) removed **4e** as a green band. The solvent was evaporated and product dissolved in small amount of ethyl acetate, then *n*-pentan was added until green crystals precipitated. The precipitate was filtered off, washed with *n*-pentane and dried *in vacuo* to afford complex **4e** (0.026 g, 25%) as a green solid. IR (KBr): ν 3080, 3059, 3027, 2976, 2926, 2854, 2506, 2313, 1939, 1835, 1731, 1683, 1620, 1604, 1585, 1526, 1495, 1460, 1421, 1406, 1382, 1373, 1332, 1296, 1253, 1200, 1173, 1157, 1136, 1112, 1046, 1033, 1008, 961, 913, 866, 826, 813, 751, 693, 649, 593, 571, 527, 494, 418 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$) δ 1.33-1.38 (m, 6H), 2.20-2.80 (m, 18H), 4.08-4.22 (m, 4H), 5.09-5.17 (m, 1H), 7.08-7.15 (m, 1H), 7.19-7.30 (m, 4H), 7.31-7.38 (m, 1H), 7.48-7.55 (m, 1H), 7.58-7.65 (m, 1H), 7.73-7.80 (m, 1H), 7.83-7.89 (m, 1H), 8.45-8.50 (m, 1H), 8.95-9.00 (m, 1H), 18.36 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 20.5, 20.6, 21.0, 21.3, 60.3, 71.7, 113.3, 121.9, 122.6, 123.2, 124.9, 126.2, 126.5, 126.8, 127.2, 127.3, 128.3, 128.6, 129.3, 131.1, 138.9, 140.0, 151.0, 211.7, 291.6. HRMS (FD/FI) calcd for $M^{+\cdot}$ ($C_{39}H_{42}N_2O^{35}Cl_2{}^{102}Ru$): 726.7; found: 727.7. Anal. Calcd. for $C_{39}H_{42}N_2OCl_2Ru$: C 64.46, H 5.83, N 3.85, Cl 9.76. Found C 64.25, H 6.05, N 3.94, Cl 9.92.

The green solid was dissolved in a small amount of ethyl acetate and *n*-pentane and left in open flask overnight at RT.

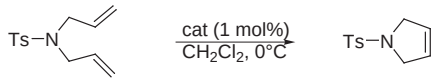
7. Reaction of complex 3a with 1-metoxybutadiene

1-Methoxy-1,3-butadiene (0.06 mL, 0.6 mmol, mixture of isomers) and CD_2Cl_2 (1.5 mL) were placed in a Schlenk flask. Afterwards carbene complex Grubbs second generation (0.051 g; 0.06 mmol) was added and the reaction mixture was kept at RT for 15.5 h. During this time ^1H NMR spectra were measured few times. After total conversion to a new complex, solvent was evaporated and residual orange powder (0.030 g) was washed with cold pentane and methanol. IR (film in DCM): ν 3386, 2927, 2851, 2740, 1980, 1940, 1726, 1685, 1631, 1607, 1480, 1443, 1380, 1327, 1266, 1214, 1175, 1130, 1037, 1005, 916, 890, 850, 802, 734, 701, 627, 579, 542, 512, 488, 448, 420, 408 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$) δ 1.00-1.15 (m, 17H), 1.55-1.74 (m, 16H) 2.22-2.32 (m, 6H), 2.48-2.52 (m, 6H), 2.60 (s, 7H), 3.30 (s, 4H), 3.85-4.05 (m, 1H), 6.90-7.00 (m, 5H), 13.57 (s, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 18.9, 19.7, 21.1, 26.1, 26.3, 26.4, 27.7, 27.8, 29.0, 29.4, 31.2, 31.4, 51.5, 51.7, 52.0, 66.4, 129.3, 129.5, 129.7, 130.0, 134.5, 136.4, 137.4, 137.6, 138.3, 138.4, 138.7, 138.8, 138.9, 220.5, 279.3. HRMS (FD/FI) calcd for $M^{+\cdot}$ ($C_{41}H_{63}N_2O^{35}Cl_2P^{102}Ru$): 802.9; found: 802.6.

8. Activity studies

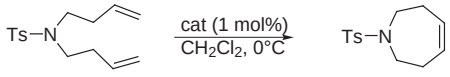
At **0 °C**: Two sets of RCM reactions were used as a test to compare the activity of catalysts: cyclization of *N*,*N*-diallyltosylamine and *N*,*N*-di(3-buten-1-yl)tosylamine in CH_2Cl_2 at 0 °C. Typically 1 mol% of the catalyst (0.004 mmol) was added to solution of a substrate (0.350 mmol) and an internal standard in 17.5

mL CH_2Cl_2 at 0 °C. The reaction was running at 0 °C under argon and samples were taken after 5 min, 10 min, 20 min, 30 min, 45 min, 60 min, 2 h, 4h, 6h and analyzed by GC. Results are presented in Tables 1 and 2.



Time [h]	Complex 3a	Complex 3b	Complex 4b	Complex 4d
0	0	0	0	0
0.17	2.1	15	4	0
0.33	5	33	7	0
0.5	7	45	9	0.9
0.75	9	59	11	2.5
1	11.5	87	14	5
1.5	15	94	18	9
2	25	96	29	19
4	45	99	48	28
6	50	99	52	31

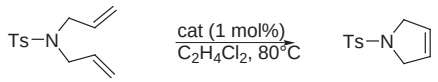
Table 1. Kinetic measurements (conversions) of RCM reaction of *N*,*N*-diallyltosylamine in CH_2Cl_2 at 0 °C (presented as a plot in article).



Time [h]	Complex 3a	Complex 3b	Complex 4b	Complex 4d
0	0	0	0	0
0.17	29	98	35	4.7
0.5	41	98	57	11.5
1	56	98	70	22
2	71	98	82	31
3	82	98	93	40
4	92	98	98	51

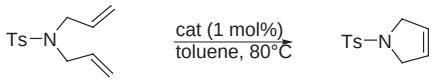
Table 2. Kinetic measurements (conversions) of RCM reaction of *N*,*N*-di(3-buten-1-yl)tosylamine in CH_2Cl_2 at 0 °C.

At **80 °C**: Two sets of RCM reactions were used as a test to compare the activity of of catalysts: cyclization of *N*,*N*-diallyltosylamine in $C_2H_4Cl_2$ and in toluene at 80 °C. Typically 1 mol% of the catalyst (0.004 mmol) was added to solution of a substrate (0.350 mmol) and an internal standard in 17.5 mL of solvent at 80 °C. The reaction was running at 80 °C under argon and samples were taken after 1 h, 2 h, 3 h, 4 h, 5 h, 6 h and analyzed by GC. Results are presented in Tables 3 and 4.



Time [h]	Complex 3a	Complex 4a	Complex 4c	Complex 4e
0	0	0	0	0
1	97	0	0	13
2	97	0	0	23
3	97	0	0	39
4	97	0	0	47
5	97	0.5	0.3	53
6	97	2.4	1	58

Table 3. Kinetic measurements (conversions) of RCM reaction of *N*,*N*-diallyltosylamine in $C_2H_4Cl_2$ at 80 °C (presented as a plot in article).



Time [h]	Complex 3a	Complex 4a	Complex 4c	Complex 4e
0	0	0	0	0
1	97	0	0	10
2	97	0	0	23
3	97	0	0	33
4	97	0.2	0	29
5	97	0.9	0.4	32
6	97	3.3	2.9	59

Table 4. Kinetic measurements (conversions) of RCM reaction of *N*,*N*-diallyltosylamine in toluene at 80 °C.

At **110 °C** (1 mol%): 1 mol% of the catalyst (0.004 mmol, 2.4 mg) was added to the solution of substrate (diethyl diallylmalonate) (0.350 mmol) and an internal standard in 17.5 mL of toluene at RT. The reaction mixture was put to the oil bath at 120 °C and refluxed under argon atmosphere for 6h and samples were taken for GC after: 15 min, 30 min, 1h, 2h, 3h, 4h, 5h and 6 hour(s).

At **110 °C** (2.5 mol%): 2.5 mol% of the catalyst (0.005 mmol, 3.0 mg) was added to the solution of substrate (diethyl diallylmalonate) (0.180 mmol) and an internal standard in 9 mL of toluene at RT. The reaction mixture was put to the oil bath at 120 °C and refluxed under argon atmosphere for 24h and samples were taken for GC after: 5 min, 10 min, 15 min, 20 min, 30 min, 1, 2, 3, 4, 5, 6 and 24 hour(s).

Results are presented in Table 5.

Time [h]	Complex 4a (1 mol%)	Complex 4c (1 mol%)	Complex 4a (2.5 mol%)	Complex 4c (2.5 mol%)
0	0	0	0	0
0.5	2.5	1.7	7.5	6.4
1	15	13.4	27	26.5

Time [h]	**Complex 4a** (1 mol%)	**Complex 4c** (1 mol%)	**Complex 4a** (2.5 mol%)	**Complex 4c** (2.5 mol%)
2	31	28.5	46.8	44.1
3	42	39.6	54.9	53
4	47	45.9	58.5	56.9
5	47.9	46.6	60.8	58.6
6	48.5	46.8	61.1	59
24	-	-	62.3	59.7

Table 5. Kinetic measurements (conversions) of RCM reaction of diethyl diallylmalonate in toluene at 110 °C.

9. ORTEPs and key details of the X-ray structures

9.1. General information

The crystal structures have been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition numbers: CCDC 698596 (**3b**), CCDC 698342 (**4a**), CCDC 698343 (**4b**), CCDC 698344 (**4d**) and CCDC 698345 (**4e**).

9.2. Experimental details of single crystal X-ray data collection

The structures of **3b**, **4a** and **4b** complexes were determined in single-crystal X-ray diffraction experiments on a Kuma KM4CCD κ-axis diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.71073 A, 45.0 kV, 40.0 mA) at 230K and 100K respectively, using the Oxford Cryostream cooling device. The crystals were mounted on thin glas rods with silicone grease and immediately cooled. Data reduction and analysis were carried out with the Kuma Diffraction programs.[5,6] The data for **4d** and **4e** were collected using the BRUKER KAPPA APEXII ULTRA controlled by APEXII software,[7] equipped with MoKα rotating anode X-ray source ($\lambda = 0.71073$ A, 50.0 kV, 100.0 mA) monochromatized by graphite monochromator and APEX-II CCD detector. The experiments were carried out at 100K using the Oxford Cryostream cooling device. The crystals were mounted on thin cactus needles with a droplet of Pantone-N oil and immediately cooled. Indexing, integration and initial scaling were performed with SAINT[8] and SADABS[9] software (Bruker, 2007). The data collection and processing statistics are reported in tables for according structures.

The structures were solved by direct methods approach using the SHELXS-97[10] program and refined with the SHELXL-97.[11] The refinement was based on F^2 for all reflections except those with negative intensities. Weighted R factors wR and all goodness-of-fit S values were based on F^2, whereas conventional R factors were based on the amplitudes, with F set to zero for negative F^2. The $F_0^2 > 2\sigma(F_0^2)$ criterion was applied only for R factors calculation was not relevant to the choice of reflections for the refinement. The R factors based on F^2 are for all structures about twice as large as those based on F. The hydrogen atoms were located in idealised geometrical positions. Scattering factors were taken from Tables 4.2.6.8 and 6.1.1.4 from the International Crystallographic Tables Vol.C.[12]

9.3. X-ray data of complex 3a

Complete structural data were taken from our recent report.[13]

[5] CrysAlis CCD, Oxford Diffraction Ltd., Version 1.171.28cycle2 beta (release 25-10-2005 CrysAlis171 .NET) (compiled Oct 25 2005,08:50:05)

[6] CrysAlis RED, Oxford Diffraction Ltd., Version 1.171.28cycle2 beta (release 25-10-2005 CrysAlis171 .NET) (compiled Oct 25 2005,08:50:05). Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid.

[7] APEXII-2008v1.0 Bruker Nonius 2007

[8] SAINT V7.34A Bruker Nonius 2007

[9] SADABS-2004/1 Bruker Nonius area detector scaling and absorption correction, 2007

[10] G. M. Sheldrick, Acta Crystallogr. **1990**, A46, 467-473

[11] G. M. Sheldrick, SHELXL93. Program for the Refinement of Crystal Structures., Univ. of Göttingen, Germany

[12] *International Tables for Crystallography*, Ed. A. J. C. Wilson, Kluwer: Dordrecht, **1992**, Vol.C

[13] M. Barbasiewicz, M. Bieniek, A. Michrowska, A. Szadkowska, A. Makal, K. Woźniak, K. Grela, *Adv. Synth. Catal.* **2007**, *349*, 193-203.

9.4. X-ray data of complex 3b

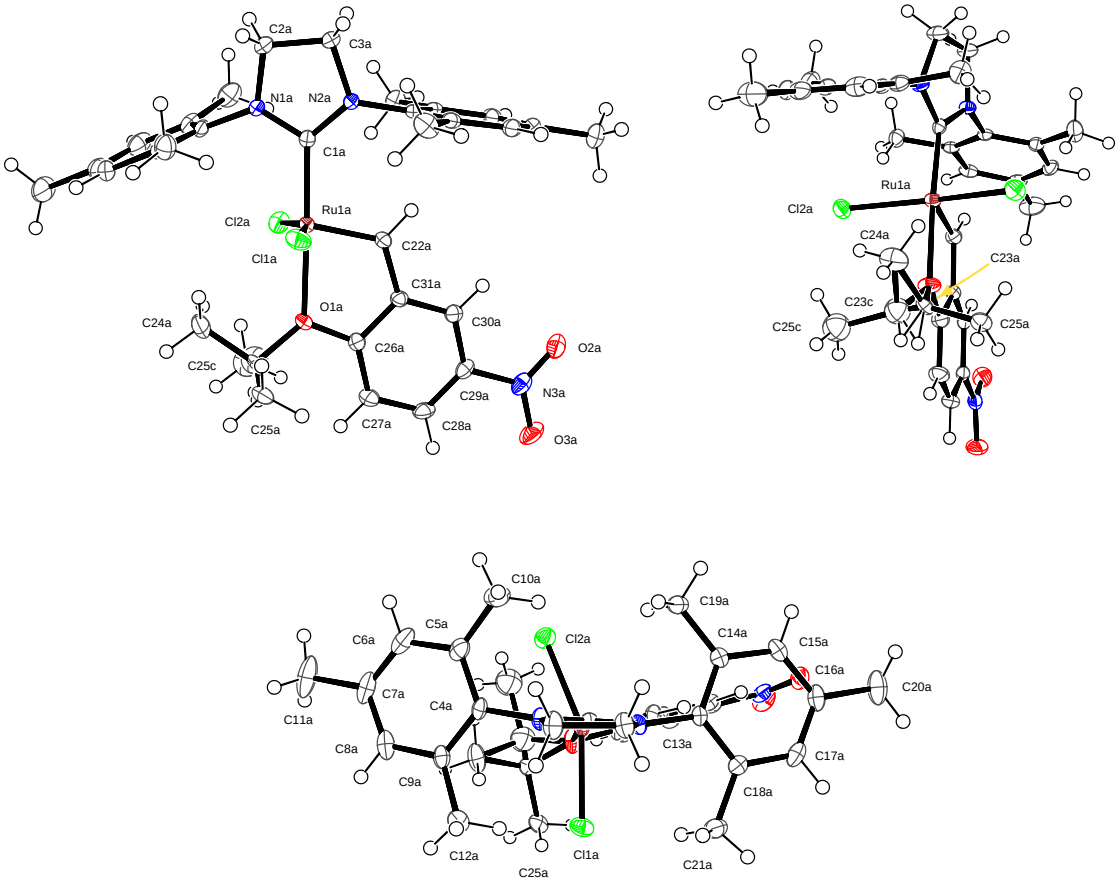


Figure 1. ORTEP[14] drawing (three orientations) of first molecule of complex **3b** present in crystal structure represented by thermal ellipsoids drawn at the 50% probability level.

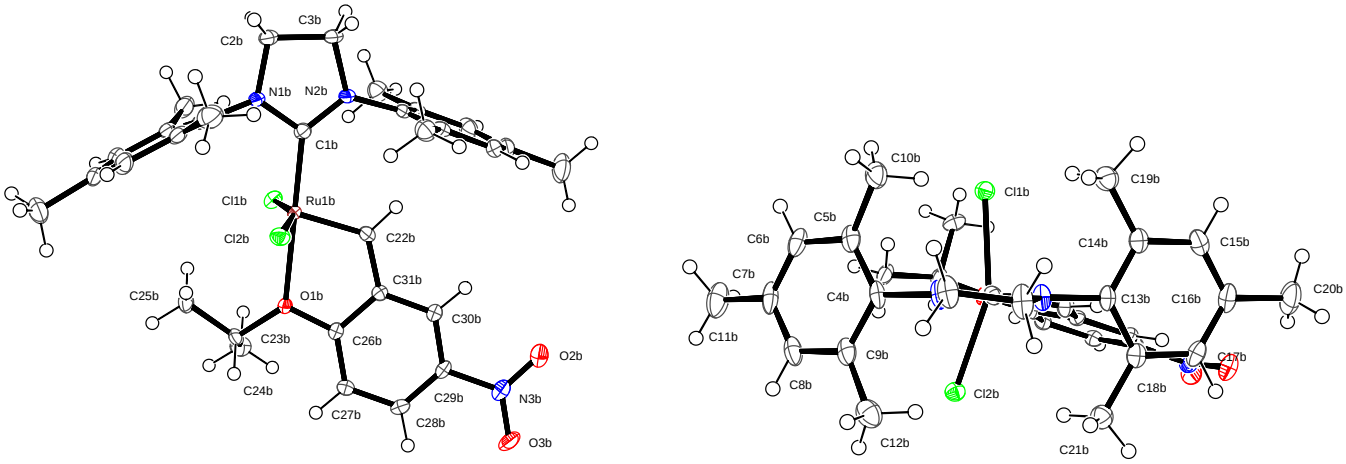


Figure 2. ORTEP drawing (two orientations) of second molecule of complex **3b** present in crystal structure represented by thermal ellipsoids drawn at the 50% probability level.

[14] We wish to acknowledge for use of a free version of Ortep-3 for Windows program: Farrugia, L. J. *J. Appl. Crystallogr.* **1997**, *30*, 565.

Table 5. Crystal data and structure refinement for complex **3b**.

Identification code	3b
Empirical formula	C62.75 H77 Cl4 N6 O7 Ru2
Formula weight	1371.24
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pbca
Unit cell dimensions	a = 22.1560(3) A alpha = 90 deg.
	b = 14.0933(2) A beta = 90 deg.
	c = 40.0696(8) A gamma = 90 deg.
Volume	12511.8(4) A^3
Z, Calculated density	8, 1.456 Mg/m^3
Absorption coefficient	0.710 mm^-1
F(000)	5660
Crystal size	0.48 x 0.20 x 0.15 mm
Theta range for data collection	2.74 to 28.79 deg.
Limiting indices	-29<=h<=29, -19<=k<=18, -54<=l<=53
Reflections collected / unique	143803 / 15676 [R(int) = 0.0280]
Completeness to theta = 28.00	99.7 %
Absorption correction	Analytical
Max. and min. transmission	0.90 and 0.75
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15676 / 35 / 772
Goodness-of-fit on F^2	1.001
Final R indices [I>2sigma(I)]	R1 = 0.0265, wR2 = 0.0678
R indices (all data)	R1 = 0.0483, wR2 = 0.0716
Largest diff. peak and hole	0.676 and -0.689 e.A^-3

Table 6. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex **3b**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ru(1A)	1363(1)	2904(1)	2864(1)	16(1)
Cl(1A)	1060(1)	1406(1)	2674(1)	26(1)
Cl(2A)	1394(1)	4234(1)	3208(1)	25(1)
O(2A)	1359(1)	5612(1)	1454(1)	29(1)
O(3A)	404(1)	5913(1)	1408(1)	35(1)
N(1A)	2221(1)	1946(1)	3305(1)	18(1)
N(2A)	2644(1)	2127(1)	2819(1)	15(1)
N(3A)	836(1)	5548(1)	1552(1)	24(1)
C(1A)	2145(1)	2340(1)	3000(1)	15(1)
C(2A)	2784(1)	1403(2)	3340(1)	24(1)
C(3A)	3097(1)	1578(2)	3009(1)	21(1)
C(4A)	1827(1)	2074(1)	3586(1)	18(1)
C(5A)	1922(1)	2858(2)	3795(1)	24(1)
C(6A)	1528(1)	2984(2)	4062(1)	31(1)
C(7A)	1066(1)	2353(2)	4131(1)	31(1)

	x	y	z	U(eq)
C(8A)	1007(1)	1560(2)	3930(1)	28(1)
C(9A)	1390(1)	1395(2)	3661(1)	20(1)
C(10A)	2446(1)	3518(2)	3744(1)	32(1)
C(11A)	648(1)	2510(2)	4425(1)	50(1)
C(12A)	1351(1)	469(2)	3475(1)	28(1)
C(13A)	2824(1)	2534(1)	2508(1)	14(1)
C(14A)	3061(1)	3453(1)	2506(1)	16(1)
C(15A)	3249(1)	3831(1)	2203(1)	19(1)
C(16A)	3213(1)	3317(2)	1907(1)	22(1)
C(17A)	2987(1)	2400(2)	1920(1)	23(1)
C(18A)	2789(1)	1991(1)	2216(1)	18(1)
C(19A)	3087(1)	4041(1)	2819(1)	22(1)
C(20A)	3408(1)	3764(2)	1583(1)	38(1)
C(21A)	2517(1)	1014(2)	2221(1)	27(1)
C(22A)	1556(1)	3492(1)	2471(1)	18(1)
O(1A)	446(1)	3437(1)	2705(1)	23(1)
C(23A)	-158(1)	3151(2)	2837(1)	16(1)
C(24A)	-37(1)	2854(2)	3194(1)	35(1)
C(25A)	-450(1)	2417(2)	2623(1)	22(1)
O(1S)	-580(2)	5529(2)	3026(1)	81(1)
C(1S)	68(2)	5629(4)	3064(1)	83(1)
O(1C)	446(1)	3437(1)	2705(1)	23(1)
C(23C)	-116(5)	3616(7)	2909(3)	41(2)
C(24C)	-37(1)	2854(2)	3194(1)	35(1)
C(25C)	-135(5)	4629(7)	3078(3)	47(2)
O(2S)	-352(5)	1763(8)	2312(3)	95(2)
C(26A)	491(1)	3974(1)	2423(1)	20(1)
C(27A)	22(1)	4453(2)	2269(1)	25(1)
C(28A)	140(1)	4978(2)	1984(1)	24(1)
C(29A)	720(1)	5008(1)	1857(1)	19(1)
C(30A)	1193(1)	4541(1)	2010(1)	18(1)
C(31A)	1086(1)	4011(1)	2295(1)	17(1)
Ru(1B)	3696(1)	6653(1)	581(1)	14(1)
Cl(1B)	3222(1)	5826(1)	1011(1)	20(1)
Cl(2B)	4465(1)	7453(1)	302(1)	19(1)
O(1B)	4270(1)	5328(1)	491(1)	16(1)
O(2B)	2995(1)	4258(1)	-838(1)	32(1)
O(3B)	3735(1)	3249(1)	-863(1)	28(1)
N(1B)	3398(1)	8474(1)	876(1)	21(1)
N(2B)	2701(1)	8147(1)	513(1)	19(1)
N(3B)	3457(1)	3895(1)	-723(1)	22(1)
C(1B)	3215(1)	7819(1)	651(1)	16(1)
C(2B)	2978(1)	9274(2)	915(1)	26(1)
C(3B)	2528(1)	9096(2)	635(1)	28(1)
C(4B)	3946(1)	8398(1)	1068(1)	21(1)
C(5B)	3946(1)	7893(2)	1367(1)	23(1)
C(6B)	4499(1)	7749(2)	1525(1)	28(1)
C(7B)	5033(1)	8117(2)	1398(1)	30(1)
C(8B)	5002(1)	8694(2)	1119(1)	30(1)
C(9B)	4464(1)	8854(2)	952(1)	25(1)
C(10B)	3374(1)	7562(2)	1533(1)	30(1)
C(11B)	5630(1)	7906(2)	1561(1)	45(1)
C(12B)	4451(1)	9542(2)	661(1)	33(1)
C(13B)	2344(1)	7681(1)	266(1)	18(1)

	x	y	z	U(eq)
C(14B)	1884(1)	7073(1)	370(1)	20(1)
C(15B)	1570(1)	6571(1)	126(1)	25(1)
C(16B)	1708(1)	6658(2)	-210(1)	26(1)
C(17B)	2159(1)	7288(1)	-305(1)	23(1)
C(18B)	2478(1)	7820(1)	-71(1)	20(1)
C(19B)	1745(1)	6946(2)	734(1)	28(1)
C(20B)	1367(1)	6089(2)	-470(1)	42(1)
C(21B)	2974(1)	8486(2)	-176(1)	26(1)
C(22B)	3317(1)	6134(1)	220(1)	18(1)
C(23B)	4717(1)	4870(1)	710(1)	18(1)
C(24B)	4436(1)	3999(2)	867(1)	25(1)
C(25B)	4898(1)	5606(2)	966(1)	24(1)
C(26B)	4105(1)	4904(1)	198(1)	15(1)
C(27B)	4393(1)	4145(1)	46(1)	16(1)
C(28B)	4176(1)	3810(1)	-257(1)	18(1)
C(29B)	3680(1)	4241(1)	-401(1)	16(1)
C(30B)	3382(1)	4989(1)	-251(1)	16(1)
C(31B)	3596(1)	5336(1)	52(1)	14(1)

Table 7. Bond lengths [Å] and angles [deg] for complex **3b**.

Ru(1A)-C(22A)	1.8286(19)	C(28A)-C(29A)	1.382(3)
Ru(1A)-C(1A)	1.9827(18)	C(28A)-H(28A)	0.9500
Ru(1A)-O(1A)	2.2581(13)	C(29A)-C(30A)	1.380(3)
Ru(1A)-Cl(2A)	2.3272(5)	C(30A)-C(31A)	1.384(3)
Ru(1A)-Cl(1A)	2.3429(5)	C(30A)-H(30A)	0.9500
O(2A)-N(3A)	1.229(2)	Ru(1B)-C(22B)	1.8251(19)
O(3A)-N(3A)	1.230(2)	Ru(1B)-C(1B)	1.9790(19)
N(1A)-C(1A)	1.355(2)	Ru(1B)-O(1B)	2.2869(12)
N(1A)-C(4A)	1.435(2)	Ru(1B)-Cl(2B)	2.3299(5)
N(1A)-C(2A)	1.471(2)	Ru(1B)-Cl(1B)	2.3330(5)
N(2A)-C(1A)	1.355(2)	O(1B)-C(26B)	1.368(2)
N(2A)-C(13A)	1.429(2)	O(1B)-C(23B)	1.473(2)
N(2A)-C(3A)	1.479(2)	O(2B)-N(3B)	1.233(2)
N(3A)-C(29A)	1.464(3)	O(3B)-N(3B)	1.234(2)
C(2A)-C(3A)	1.517(3)	N(1B)-C(1B)	1.352(2)
C(2A)-H(2A1)	0.9900	N(1B)-C(4B)	1.443(2)
C(2A)-H(2A2)	0.9900	N(1B)-C(2B)	1.469(2)
C(3A)-H(3A1)	0.9900	N(2B)-C(1B)	1.346(2)
C(3A)-H(3A2)	0.9900	N(2B)-C(13B)	1.429(2)
C(4A)-C(9A)	1.395(3)	N(2B)-C(3B)	1.473(2)
C(4A)-C(5A)	1.402(3)	N(3B)-C(29B)	1.467(2)
C(5A)-C(6A)	1.390(3)	C(2B)-C(3B)	1.521(3)
C(5A)-C(10A)	1.501(3)	C(2B)-H(2B1)	0.9900
C(6A)-C(7A)	1.385(3)	C(2B)-H(2B2)	0.9900
C(6A)-H(6A)	0.9500	C(3B)-H(3B1)	0.9900
C(7A)-C(8A)	1.384(3)	C(3B)-H(3B2)	0.9900
C(7A)-C(11A)	1.514(3)	C(4B)-C(5B)	1.394(3)
C(8A)-C(9A)	1.394(3)	C(4B)-C(9B)	1.396(3)
C(8A)-H(8A)	0.9500	C(5B)-C(6B)	1.394(3)
C(9A)-C(12A)	1.505(3)	C(5B)-C(10B)	1.506(3)
C(10A)-H(10A)	0.9800	C(6B)-C(7B)	1.389(3)
C(10A)-H(10B)	0.9800	C(6B)-H(6B)	0.9500
C(10A)-H(10C)	0.9800	C(7B)-C(8B)	1.382(3)

C(11A)-H(11A)	0.9800
C(11A)-H(11B)	0.9800
C(11A)-H(11C)	0.9800
C(12A)-H(12A)	0.9800
C(12A)-H(12B)	0.9800
C(12A)-H(12C)	0.9800
C(13A)-C(14A)	1.398(3)
C(13A)-C(18A)	1.400(3)
C(14A)-C(15A)	1.391(3)
C(14A)-C(19A)	1.503(3)
C(15A)-C(16A)	1.392(3)
C(15A)-H(15A)	0.9500
C(16A)-C(17A)	1.388(3)
C(16A)-C(20A)	1.508(3)
C(17A)-C(18A)	1.388(3)
C(17A)-H(17A)	0.9500
C(18A)-C(21A)	1.503(3)
C(19A)-H(19A)	0.9800
C(19A)-H(19B)	0.9800
C(19A)-H(19C)	0.9800
C(20A)-H(20A)	0.9800
C(20A)-H(20B)	0.9800
C(20A)-H(20C)	0.9800
C(21A)-H(21A)	0.9800
C(21A)-H(21B)	0.9800
C(21A)-H(21C)	0.9800
C(22A)-C(31A)	1.457(3)
C(22A)-H(22A)	0.9500
O(1A)-C(26A)	1.363(2)
O(1A)-C(23A)	1.496(3)
C(23A)-C(25A)	1.492(4)
C(23A)-C(24A)	1.512(3)
C(23A)-H(23A)	1.000
C(24A)-H(24A)	0.9800
C(24A)-H(24B)	0.9800
C(24A)-H(24C)	0.9800
C(25A)-H(25A)	0.9800
C(25A)-H(25B)	0.9800
C(25A)-H(25C)	0.9800
O(1S)-C(1S)	1.450(5)
O(1S)-H(1S4)	0.960(5)
C(1S)-H(1S1)	0.9800
C(1S)-H(1S2)	0.9800
C(1S)-H(1S3)	0.9800
C(23C)-C(25C)	1.580(12)
C(23C)-H(23C)	1.000
C(25C)-H(25D)	0.9800
C(25C)-H(25E)	0.9800
C(25C)-H(25F)	0.9800
C(26A)-C(27A)	1.384(3)
C(26A)-C(31A)	1.415(3)
C(27A)-C(28A)	1.385(3)
C(27A)-H(27A)	0.9500
C(7B)-C(11B)	1.507(3)
C(8B)-C(9B)	1.386(3)
C(8B)-H(8B)	0.9500
C(9B)-C(12B)	1.516(3)
C(10B)-H(10D)	0.9800
C(10B)-H(10E)	0.9800
C(10B)-H(10F)	0.9800
C(11B)-H(11D)	0.9800
C(11B)-H(11E)	0.9800
C(11B)-H(11F)	0.9800
C(12B)-H(12D)	0.9800
C(12B)-H(12E)	0.9800
C(12B)-H(12F)	0.9800
C(13B)-C(14B)	1.395(3)
C(13B)-C(18B)	1.397(3)
C(14B)-C(15B)	1.393(3)
C(14B)-C(19B)	1.501(3)
C(15B)-C(16B)	1.385(3)
C(15B)-H(15B)	0.9500
C(16B)-C(17B)	1.391(3)
C(16B)-C(20B)	1.515(3)
C(17B)-C(18B)	1.393(3)
C(17B)-H(17B)	0.9500
C(18B)-C(21B)	1.504(3)
C(19B)-H(19D)	0.9800
C(19B)-H(19E)	0.9800
C(19B)-H(19F)	0.9800
C(20B)-H(20D)	0.9800
C(20B)-H(20E)	0.9800
C(20B)-H(20F)	0.9800
C(21B)-H(21D)	0.9800
C(21B)-H(21E)	0.9800
C(21B)-H(21F)	0.9800
C(22B)-C(31B)	1.449(3)
C(22B)-H(22B)	0.9500
C(23B)-C(25B)	1.511(3)
C(23B)-C(24B)	1.513(3)
C(23B)-H(23B)	1.000
C(24B)-H(24D)	0.9800
C(24B)-H(24E)	0.9800
C(24B)-H(24F)	0.9800
C(25B)-H(25G)	0.9800
C(25B)-H(25H)	0.9800
C(25B)-H(25I)	0.9800
C(26B)-C(27B)	1.386(3)
C(26B)-C(31B)	1.407(2)
C(27B)-C(28B)	1.390(3)
C(27B)-H(27B)	0.9500
C(28B)-C(29B)	1.379(3)
C(28B)-H(28B)	0.9500
C(29B)-C(30B)	1.380(3)
C(30B)-C(31B)	1.394(3)
C(30B)-H(30B)	0.9500

C(22A)-Ru(1A)-C(1A)	102.31(8)
C(22A)-Ru(1A)-O(1A)	79.43(7)
C(1A)-Ru(1A)-O(1A)	175.80(6)
C(22A)-Ru(1A)-Cl(2A)	97.91(6)
C(1A)-Ru(1A)-Cl(2A)	97.77(5)
O(1A)-Ru(1A)-Cl(2A)	85.73(4)
C(22A)-Ru(1A)-Cl(1A)	101.32(6)
C(1A)-Ru(1A)-Cl(1A)	88.76(5)
O(1A)-Ru(1A)-Cl(1A)	87.14(4)
Cl(2A)-Ru(1A)-Cl(1A)	157.88(2)
C(1A)-N(1A)-C(4A)	125.62(16)
C(1A)-N(1A)-C(2A)	113.82(15)
C(4A)-N(1A)-C(2A)	120.43(15)
C(1A)-N(2A)-C(13A)	127.14(15)
C(1A)-N(2A)-C(3A)	113.21(15)
C(13A)-N(2A)-C(3A)	118.12(14)
O(2A)-N(3A)-O(3A)	123.52(18)
O(2A)-N(3A)-C(29A)	118.08(16)
O(3A)-N(3A)-C(29A)	118.40(18)
N(1A)-C(1A)-N(2A)	106.94(16)
N(1A)-C(1A)-Ru(1A)	121.35(13)
N(2A)-C(1A)-Ru(1A)	130.94(14)
N(1A)-C(2A)-C(3A)	102.73(15)
N(1A)-C(2A)-H(2A1)	111.2
C(3A)-C(2A)-H(2A1)	111.2
N(1A)-C(2A)-H(2A2)	111.2
C(3A)-C(2A)-H(2A2)	111.2
H(2A1)-C(2A)-H(2A2)	109.1
N(2A)-C(3A)-C(2A)	103.02(15)
N(2A)-C(3A)-H(3A1)	111.2
C(2A)-C(3A)-H(3A1)	111.2
N(2A)-C(3A)-H(3A2)	111.2
C(2A)-C(3A)-H(3A2)	111.2
H(3A1)-C(3A)-H(3A2)	109.1
C(9A)-C(4A)-C(5A)	121.15(18)
C(9A)-C(4A)-N(1A)	120.24(18)
C(5A)-C(4A)-N(1A)	118.46(18)
C(6A)-C(5A)-C(4A)	117.7(2)
C(6A)-C(5A)-C(10A)	120.7(2)
C(4A)-C(5A)-C(10A)	121.53(19)
C(7A)-C(6A)-C(5A)	122.5(2)
C(7A)-C(6A)-H(6A)	118.7
C(5A)-C(6A)-H(6A)	118.7
C(8A)-C(7A)-C(6A)	118.1(2)
C(8A)-C(7A)-C(11A)	120.8(2)
C(6A)-C(7A)-C(11A)	121.1(2)
C(7A)-C(8A)-C(9A)	121.9(2)
C(7A)-C(8A)-H(8A)	119.1
C(9A)-C(8A)-H(8A)	119.1
C(8A)-C(9A)-C(4A)	118.3(2)
C(8A)-C(9A)-C(12A)	119.58(19)
C(4A)-C(9A)-C(12A)	121.93(18)
C(5A)-C(10A)-H(10A)	109.5
C(5A)-C(10A)-H(10B)	109.5
H(10A)-C(10A)-H(10B)	109.5
C(1B)-Ru(1B)-O(1B)	178.45(7)
C(22B)-Ru(1B)-Cl(2B)	98.67(6)
C(1B)-Ru(1B)-Cl(2B)	93.43(5)
O(1B)-Ru(1B)-Cl(2B)	85.03(3)
C(22B)-Ru(1B)-Cl(1B)	100.31(6)
C(1B)-Ru(1B)-Cl(1B)	93.86(6)
O(1B)-Ru(1B)-Cl(1B)	87.64(3)
Cl(2B)-Ru(1B)-Cl(1B)	157.880(18)
C(26B)-O(1B)-C(23B)	120.06(14)
C(26B)-O(1B)-Ru(1B)	110.07(10)
C(23B)-O(1B)-Ru(1B)	129.60(10)
C(1B)-N(1B)-C(4B)	123.84(16)
C(1B)-N(1B)-C(2B)	113.95(15)
C(4B)-N(1B)-C(2B)	122.20(15)
C(1B)-N(2B)-C(13B)	126.44(16)
C(1B)-N(2B)-C(3B)	113.39(16)
C(13B)-N(2B)-C(3B)	120.14(15)
O(2B)-N(3B)-O(3B)	123.36(17)
O(2B)-N(3B)-C(29B)	118.14(16)
O(3B)-N(3B)-C(29B)	118.50(17)
N(2B)-C(1B)-N(1B)	106.88(16)
N(2B)-C(1B)-Ru(1B)	133.05(14)
N(1B)-C(1B)-Ru(1B)	120.07(13)
N(1B)-C(2B)-C(3B)	102.08(15)
N(1B)-C(2B)-H(2B1)	111.4
C(3B)-C(2B)-H(2B1)	111.4
N(1B)-C(2B)-H(2B2)	111.4
C(3B)-C(2B)-H(2B2)	111.4
H(2B1)-C(2B)-H(2B2)	109.2
N(2B)-C(3B)-C(2B)	102.85(16)
N(2B)-C(3B)-H(3B1)	111.2
C(2B)-C(3B)-H(3B1)	111.2
N(2B)-C(3B)-H(3B2)	111.2
C(2B)-C(3B)-H(3B2)	111.2
H(3B1)-C(3B)-H(3B2)	109.1
C(5B)-C(4B)-C(9B)	121.45(18)
C(5B)-C(4B)-N(1B)	119.86(18)
C(9B)-C(4B)-N(1B)	118.68(19)
C(4B)-C(5B)-C(6B)	117.7(2)
C(4B)-C(5B)-C(10B)	122.61(19)
C(6B)-C(5B)-C(10B)	119.5(2)
C(7B)-C(6B)-C(5B)	121.8(2)
C(7B)-C(6B)-H(6B)	119.1
C(5B)-C(6B)-H(6B)	119.1
C(8B)-C(7B)-C(6B)	118.29(19)
C(8B)-C(7B)-C(11B)	120.8(2)
C(6B)-C(7B)-C(11B)	120.9(2)
C(7B)-C(8B)-C(9B)	122.0(2)
C(7B)-C(8B)-H(8B)	119.0
C(9B)-C(8B)-H(8B)	119.0
C(8B)-C(9B)-C(4B)	118.1(2)
C(8B)-C(9B)-C(12B)	119.4(2)
C(4B)-C(9B)-C(12B)	122.42(19)
C(5B)-C(10B)-H(10D)	109.5
C(5B)-C(10B)-H(10E)	109.5

C(5A)-C(10A)-H(10C)	109.5
H(10A)-C(10A)-H(10C)	109.5
H(10B)-C(10A)-H(10C)	109.5
C(7A)-C(11A)-H(11A)	109.5
C(7A)-C(11A)-H(11B)	109.5
H(11A)-C(11A)-H(11B)	109.5
C(7A)-C(11A)-H(11C)	109.5
H(11A)-C(11A)-H(11C)	109.5
H(11B)-C(11A)-H(11C)	109.5
C(9A)-C(12A)-H(12A)	109.5
C(9A)-C(12A)-H(12B)	109.5
H(12A)-C(12A)-H(12B)	109.5
C(9A)-C(12A)-H(12C)	109.5
H(12A)-C(12A)-H(12C)	109.5
H(12B)-C(12A)-H(12C)	109.5
C(14A)-C(13A)-C(18A)	121.55(17)
C(14A)-C(13A)-N(2A)	118.78(16)
C(18A)-C(13A)-N(2A)	119.58(17)
C(15A)-C(14A)-C(13A)	118.14(18)
C(15A)-C(14A)-C(19A)	120.40(17)
C(13A)-C(14A)-C(19A)	121.40(17)
C(14A)-C(15A)-C(16A)	121.91(19)
C(14A)-C(15A)-H(15A)	119.0
C(16A)-C(15A)-H(15A)	119.0
C(17A)-C(16A)-C(15A)	118.16(18)
C(17A)-C(16A)-C(20A)	121.8(2)
C(15A)-C(16A)-C(20A)	120.1(2)
C(16A)-C(17A)-C(18A)	122.30(19)
C(16A)-C(17A)-H(17A)	118.9
C(18A)-C(17A)-H(17A)	118.9
C(17A)-C(18A)-C(13A)	117.92(18)
C(17A)-C(18A)-C(21A)	121.24(18)
C(13A)-C(18A)-C(21A)	120.77(18)
C(14A)-C(19A)-H(19A)	109.5
C(14A)-C(19A)-H(19B)	109.5
H(19A)-C(19A)-H(19B)	109.5
C(14A)-C(19A)-H(19C)	109.5
H(19A)-C(19A)-H(19C)	109.5
H(19B)-C(19A)-H(19C)	109.5
C(16A)-C(20A)-H(20A)	109.5
C(16A)-C(20A)-H(20B)	109.5
H(20A)-C(20A)-H(20B)	109.5
C(16A)-C(20A)-H(20C)	109.5
H(20A)-C(20A)-H(20C)	109.5
H(20B)-C(20A)-H(20C)	109.5
C(18A)-C(21A)-H(21A)	109.5
C(18A)-C(21A)-H(21B)	109.5
H(21A)-C(21A)-H(21B)	109.5
C(18A)-C(21A)-H(21C)	109.5
H(21A)-C(21A)-H(21C)	109.5
H(21B)-C(21A)-H(21C)	109.5
C(31A)-C(22A)-Ru(1A)	118.50(14)
C(31A)-C(22A)-H(22A)	120.7
Ru(1A)-C(22A)-H(22A)	120.7
C(26A)-O(1A)-C(23A)	120.65(16)
H(10D)-C(10B)-H(10E)	109.5
C(5B)-C(10B)-H(10F)	109.5
H(10D)-C(10B)-H(10F)	109.5
H(10E)-C(10B)-H(10F)	109.5
C(7B)-C(11B)-H(11D)	109.5
C(7B)-C(11B)-H(11E)	109.5
H(11D)-C(11B)-H(11E)	109.5
C(7B)-C(11B)-H(11F)	109.5
H(11D)-C(11B)-H(11F)	109.5
H(11E)-C(11B)-H(11F)	109.5
C(9B)-C(12B)-H(12D)	109.5
C(9B)-C(12B)-H(12E)	109.5
H(12D)-C(12B)-H(12E)	109.5
C(9B)-C(12B)-H(12F)	109.5
H(12D)-C(12B)-H(12F)	109.5
H(12E)-C(12B)-H(12F)	109.5
C(14B)-C(13B)-C(18B)	122.05(18)
C(14B)-C(13B)-N(2B)	118.72(18)
C(18B)-C(13B)-N(2B)	119.19(18)
C(15B)-C(14B)-C(13B)	117.83(19)
C(15B)-C(14B)-C(19B)	121.30(19)
C(13B)-C(14B)-C(19B)	120.85(18)
C(16B)-C(15B)-C(14B)	121.8(2)
C(16B)-C(15B)-H(15B)	119.1
C(14B)-C(15B)-H(15B)	119.1
C(15B)-C(16B)-C(17B)	118.67(19)
C(15B)-C(16B)-C(20B)	120.7(2)
C(17B)-C(16B)-C(20B)	120.6(2)
C(16B)-C(17B)-C(18B)	121.7(2)
C(16B)-C(17B)-H(17B)	119.1
C(18B)-C(17B)-H(17B)	119.1
C(17B)-C(18B)-C(13B)	117.77(19)
C(17B)-C(18B)-C(21B)	121.27(19)
C(13B)-C(18B)-C(21B)	120.88(18)
C(14B)-C(19B)-H(19D)	109.5
C(14B)-C(19B)-H(19E)	109.5
H(19D)-C(19B)-H(19E)	109.5
C(14B)-C(19B)-H(19F)	109.5
H(19D)-C(19B)-H(19F)	109.5
H(19E)-C(19B)-H(19F)	109.5
C(16B)-C(20B)-H(20D)	109.5
C(16B)-C(20B)-H(20E)	109.5
H(20D)-C(20B)-H(20E)	109.5
C(16B)-C(20B)-H(20F)	109.5
H(20D)-C(20B)-H(20F)	109.5
H(20E)-C(20B)-H(20F)	109.5
C(18B)-C(21B)-H(21D)	109.5
C(18B)-C(21B)-H(21E)	109.5
H(21D)-C(21B)-H(21E)	109.5
C(18B)-C(21B)-H(21F)	109.5
H(21D)-C(21B)-H(21F)	109.5
H(21E)-C(21B)-H(21F)	109.5
C(31B)-C(22B)-Ru(1B)	118.73(14)
C(31B)-C(22B)-H(22B)	120.6
Ru(1B)-C(22B)-H(22B)	120.6

C(26A)-O(1A)-Ru(1A)	110.73(11)	O(1B)-C(23B)-C(25B)	106.35(15)
C(23A)-O(1A)-Ru(1A)	127.89(13)	O(1B)-C(23B)-C(24B)	109.00(15)
C(25A)-C(23A)-O(1A)	111.7(2)	C(25B)-C(23B)-C(24B)	112.67(17)
C(25A)-C(23A)-C(24A)	115.4(2)	O(1B)-C(23B)-H(23B)	109.6
O(1A)-C(23A)-C(24A)	104.63(18)	C(25B)-C(23B)-H(23B)	109.6
C(25A)-C(23A)-H(23A)	108.3	C(24B)-C(23B)-H(23B)	109.6
O(1A)-C(23A)-H(23A)	108.3	C(23B)-C(24B)-H(24D)	109.5
C(24A)-C(23A)-H(23A)	108.3	C(23B)-C(24B)-H(24E)	109.5
C(1S)-O(1S)-H(1S4)	112(3)	H(24D)-C(24B)-H(24E)	109.5
C(25C)-C(23C)-H(23C)	111.3	C(23B)-C(24B)-H(24F)	109.5
C(23C)-C(25C)-H(25D)	109.5	H(24D)-C(24B)-H(24F)	109.5
C(23C)-C(25C)-H(25E)	109.5	H(24E)-C(24B)-H(24F)	109.5
H(25D)-C(25C)-H(25E)	109.5	C(23B)-C(25B)-H(25G)	109.5
C(23C)-C(25C)-H(25F)	109.5	C(23B)-C(25B)-H(25H)	109.5
H(25D)-C(25C)-H(25F)	109.5	H(25G)-C(25B)-H(25H)	109.5
H(25E)-C(25C)-H(25F)	109.5	C(23B)-C(25B)-H(25I)	109.5
O(1A)-C(26A)-C(27A)	125.85(18)	H(25G)-C(25B)-H(25I)	109.5
O(1A)-C(26A)-C(31A)	112.79(16)	H(25H)-C(25B)-H(25I)	109.5
C(27A)-C(26A)-C(31A)	121.35(18)	O(1B)-C(26B)-C(27B)	126.18(17)
C(26A)-C(27A)-C(28A)	119.06(19)	O(1B)-C(26B)-C(31B)	112.34(16)
C(26A)-C(27A)-H(27A)	120.5	C(27B)-C(26B)-C(31B)	121.47(17)
C(28A)-C(27A)-H(27A)	120.5	C(26B)-C(27B)-C(28B)	119.00(18)
C(29A)-C(28A)-C(27A)	119.62(18)	C(26B)-C(27B)-H(27B)	120.5
C(29A)-C(28A)-H(28A)	120.2	C(28B)-C(27B)-H(27B)	120.5
C(27A)-C(28A)-H(28A)	120.2	C(29B)-C(28B)-C(27B)	119.40(17)
C(30A)-C(29A)-C(28A)	121.89(19)	C(29B)-C(28B)-H(28B)	120.3
C(30A)-C(29A)-N(3A)	119.14(18)	C(27B)-C(28B)-H(28B)	120.3
C(28A)-C(29A)-N(3A)	118.97(17)	C(28B)-C(29B)-C(30B)	122.43(17)
C(29A)-C(30A)-C(31A)	119.57(18)	C(28B)-C(29B)-N(3B)	119.30(17)
C(29A)-C(30A)-H(30A)	120.2	C(30B)-C(29B)-N(3B)	118.27(17)
C(31A)-C(30A)-H(30A)	120.2	C(29B)-C(30B)-C(31B)	118.93(18)
C(30A)-C(31A)-C(26A)	118.50(17)	C(29B)-C(30B)-H(30B)	120.5
C(30A)-C(31A)-C(22A)	123.26(17)	C(31B)-C(30B)-H(30B)	120.5
C(26A)-C(31A)-C(22A)	118.24(17)	C(30B)-C(31B)-C(26B)	118.75(17)
C(22B)-Ru(1B)-C(1B)	101.36(8)	C(30B)-C(31B)-C(22B)	122.10(17)
C(22B)-Ru(1B)-O(1B)	78.74(7)	C(26B)-C(31B)-C(22B)	119.14(17)

Table 8. Anisotropic displacement parameters ($A^2 \times 10^3$) for complex **3b**. The anisotropic displacement factor exponent takes the form: $-2\,\pi^2 \times [h^2 \times a^2 \times U_{11} + ... + 2 \times h \times k \times a \times b \times U_{12}]$

	$\mathbf{U}_{11}$	$\mathbf{U}_{22}$	$\mathbf{U}_{33}$	$\mathbf{U}_{23}$	$\mathbf{U}_{13}$	$\mathbf{U}_{12}$
Ru(1A)	14(1)	18(1)	15(1)	2(1)	1(1)	1(1)
Cl(1A)	18(1)	24(1)	35(1)	-2(1)	-2(1)	-3(1)
Cl(2A)	32(1)	21(1)	24(1)	-1(1)	1(1)	4(1)
O(2A)	38(1)	30(1)	20(1)	4(1)	3(1)	2(1)
O(3A)	43(1)	36(1)	25(1)	6(1)	-8(1)	17(1)
N(1A)	17(1)	22(1)	14(1)	4(1)	1(1)	3(1)
N(2A)	14(1)	16(1)	15(1)	4(1)	1(1)	2(1)
N(3A)	36(1)	20(1)	18(1)	-3(1)	-3(1)	7(1)
C(1A)	16(1)	14(1)	14(1)	-1(1)	-1(1)	-3(1)
C(2A)	23(1)	31(1)	20(1)	8(1)	0(1)	8(1)

	$\mathbf{U}_{11}$	$\mathbf{U}_{22}$	$\mathbf{U}_{33}$	$\mathbf{U}_{23}$	$\mathbf{U}_{13}$	$\mathbf{U}_{12}$
C(3A)	18(1)	27(1)	20(1)	7(1)	-1(1)	4(1)
C(4A)	21(1)	21(1)	11(1)	3(1)	1(1)	5(1)
C(5A)	31(1)	23(1)	16(1)	2(1)	-5(1)	4(1)
C(6A)	44(1)	31(1)	17(1)	-5(1)	-4(1)	14(1)
C(7A)	31(1)	46(1)	15(1)	3(1)	3(1)	19(1)
C(8A)	22(1)	42(1)	21(1)	10(1)	5(1)	4(1)
C(9A)	20(1)	26(1)	15(1)	6(1)	0(1)	2(1)
C(10A)	41(1)	28(1)	27(1)	-2(1)	-8(1)	-5(1)
C(11A)	48(2)	79(2)	23(1)	7(1)	14(1)	33(2)
C(12A)	30(1)	26(1)	26(1)	2(1)	2(1)	-6(1)
C(13A)	11(1)	18(1)	13(1)	3(1)	0(1)	3(1)
C(14A)	11(1)	18(1)	19(1)	2(1)	-1(1)	3(1)
C(15A)	14(1)	20(1)	25(1)	8(1)	1(1)	2(1)
C(16A)	17(1)	32(1)	18(1)	9(1)	1(1)	5(1)
C(17A)	19(1)	35(1)	15(1)	-4(1)	-2(1)	7(1)
C(18A)	13(1)	21(1)	19(1)	-2(1)	-2(1)	3(1)
C(19A)	26(1)	19(1)	22(1)	-2(1)	-2(1)	-4(1)
C(20A)	37(1)	55(2)	24(1)	17(1)	7(1)	7(1)
C(21A)	26(1)	25(1)	31(1)	-9(1)	2(1)	-2(1)
C(22A)	14(1)	22(1)	17(1)	-1(1)	2(1)	2(1)
O(1A)	13(1)	35(1)	21(1)	6(1)	3(1)	5(1)
C(23A)	9(1)	16(1)	22(2)	-1(1)	6(1)	2(1)
C(24A)	26(1)	44(2)	34(1)	11(1)	13(1)	5(1)
C(25A)	13(1)	23(1)	30(2)	1(1)	2(1)	-1(1)
O(1S)	84(2)	76(2)	82(2)	12(2)	1(2)	7(2)
C(1S)	85(3)	85(3)	78(3)	-16(2)	-18(2)	28(2)
O(1C)	13(1)	35(1)	21(1)	6(1)	3(1)	5(1)
C(24C)	26(1)	44(2)	34(1)	11(1)	13(1)	5(1)
C(26A)	18(1)	27(1)	16(1)	0(1)	2(1)	4(1)
C(27A)	17(1)	33(1)	25(1)	0(1)	2(1)	8(1)
C(28A)	22(1)	26(1)	24(1)	-2(1)	-5(1)	10(1)
C(29A)	27(1)	16(1)	15(1)	-3(1)	-3(1)	4(1)
C(30A)	19(1)	19(1)	16(1)	-4(1)	-1(1)	2(1)
C(31A)	16(1)	20(1)	17(1)	-2(1)	-1(1)	3(1)
Ru(1B)	13(1)	14(1)	13(1)	-3(1)	-1(1)	2(1)
Cl(1B)	23(1)	19(1)	19(1)	-3(1)	2(1)	-2(1)
Cl(2B)	18(1)	20(1)	19(1)	0(1)	2(1)	2(1)
O(1B)	19(1)	17(1)	13(1)	-2(1)	-3(1)	4(1)
O(2B)	37(1)	36(1)	23(1)	-5(1)	-9(1)	5(1)
O(3B)	31(1)	31(1)	22(1)	-13(1)	5(1)	0(1)
N(1B)	15(1)	19(1)	29(1)	-12(1)	-6(1)	5(1)
N(2B)	17(1)	15(1)	24(1)	-7(1)	-5(1)	5(1)
N(3B)	25(1)	24(1)	17(1)	-4(1)	1(1)	-5(1)
C(1B)	14(1)	17(1)	18(1)	-2(1)	1(1)	-1(1)
C(2B)	21(1)	22(1)	36(1)	-14(1)	-6(1)	6(1)
C(3B)	24(1)	21(1)	38(1)	-15(1)	-9(1)	10(1)
C(4B)	13(1)	22(1)	27(1)	-13(1)	-5(1)	4(1)
C(5B)	20(1)	26(1)	25(1)	-14(1)	-1(1)	4(1)
C(6B)	28(1)	37(1)	19(1)	-12(1)	-6(1)	8(1)
C(7B)	19(1)	44(1)	28(1)	-23(1)	-7(1)	8(1)
C(8B)	15(1)	43(1)	32(1)	-19(1)	0(1)	-2(1)
C(9B)	21(1)	28(1)	25(1)	-16(1)	0(1)	1(1)
C(10B)	29(1)	35(1)	28(1)	-11(1)	0(1)	-4(1)
C(11B)	24(1)	72(2)	38(2)	-18(1)	-10(1)	11(1)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(12B)	30(1)	31(1)	39(1)	-8(1)	3(1)	-2(1)
C(13B)	16(1)	15(1)	22(1)	-5(1)	-7(1)	6(1)
C(14B)	17(1)	19(1)	25(1)	-1(1)	-4(1)	6(1)
C(15B)	20(1)	19(1)	35(1)	0(1)	-8(1)	-2(1)
C(16B)	30(1)	20(1)	28(1)	-4(1)	-14(1)	5(1)
C(17B)	27(1)	23(1)	19(1)	-2(1)	-7(1)	8(1)
C(18B)	18(1)	18(1)	24(1)	-2(1)	-4(1)	7(1)
C(19B)	25(1)	30(1)	28(1)	1(1)	0(1)	1(1)
C(20B)	53(2)	37(1)	36(1)	-5(1)	-22(1)	-8(1)
C(21B)	23(1)	28(1)	25(1)	0(1)	-1(1)	1(1)
C(22B)	16(1)	17(1)	20(1)	-1(1)	-3(1)	4(1)
C(23B)	16(1)	22(1)	15(1)	2(1)	-3(1)	5(1)
C(24B)	31(1)	24(1)	21(1)	7(1)	3(1)	3(1)
C(25B)	23(1)	34(1)	15(1)	-1(1)	-5(1)	2(1)
C(26B)	16(1)	15(1)	13(1)	0(1)	0(1)	-3(1)
C(27B)	15(1)	16(1)	18(1)	0(1)	1(1)	1(1)
C(28B)	19(1)	15(1)	19(1)	-3(1)	5(1)	-1(1)
C(29B)	20(1)	16(1)	12(1)	-3(1)	1(1)	-4(1)
C(30B)	17(1)	15(1)	14(1)	0(1)	0(1)	-2(1)
C(31B)	16(1)	13(1)	14(1)	1(1)	1(1)	0(1)

Table 9. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($A^2 \times 10^3$) for complex **3b**.

	x	**y**	**z**	**U(eq)**
H(2A1)	2701	719	3373	29
H(2A2)	3029	1640	3529	29
H(3A1)	3473	1948	3040	26
H(3A2)	3195	973	2896	26
H(6A)	1578	3523	4201	37
H(8A)	697	1114	3978	34
H(10A)	2389	4088	3881	48
H(10B)	2470	3698	3508	48
H(10C)	2820	3199	3811	48
H(11A)	228	2448	4351	75
H(11B)	713	3147	4516	75
H(11C)	732	2036	4598	75
H(12A)	1367	590	3234	41
H(12B)	971	150	3530	41
H(12C)	1691	63	3539	41
H(15A)	3407	4458	2198	23
H(17A)	2968	2039	1720	27
H(19A)	3296	4639	2772	34
H(19B)	3306	3692	2992	34
H(19C)	2676	4175	2896	34
H(20A)	3485	3266	1417	57
H(20B)	3779	4131	1618	57
H(20C)	3089	4186	1501	57
H(21A)	2502	762	1993	41
H(21B)	2107	1047	2312	41

	x	y	z	U(eq)
H(21C)	2764	597	2361	41
H(22A)	1955	3459	2384	21
H(23A)	-423	3724	2841	19
H(24A)	203	2269	3195	52
H(24B)	-421	2742	3308	52
H(24C)	186	3357	3309	52
H(25A)	-480	2653	2394	33
H(25B)	-854	2278	2709	33
H(25C)	-206	1836	2626	33
H(1S4)	-733(18)	5890(30)	2840(7)	80
H(1S1)	264	5541	2847	124
H(1S2)	217	5149	3220	124
H(1S3)	161	6263	3150	124
H(23C)	-490	3494	2775	49
H(25D)	215	4703	3225	71
H(25E)	-507	4693	3208	71
H(25F)	-125	5120	2905	71
H(27A)	-375	4423	2357	30
H(28A)	-176	5315	1876	28
H(30A)	1589	4583	1921	22
H(2B1)	3187	9889	886	32
H(2B2)	2778	9261	1136	32
H(3B1)	2109	9099	719	33
H(3B2)	2568	9578	456	33
H(6B)	4511	7390	1726	34
H(8B)	5359	8990	1040	36
H(10D)	3250	8027	1702	46
H(10E)	3445	6947	1641	46
H(10F)	3055	7496	1366	46
H(11D)	5767	7272	1495	67
H(11E)	5584	7929	1804	67
H(11F)	5929	8378	1491	67
H(12D)	4120	9374	510	50
H(12E)	4835	9509	540	50
H(12F)	4391	10188	745	50
H(15B)	1253	6157	192	30
H(17B)	2253	7357	-535	27
H(19D)	2084	6629	844	41
H(19E)	1380	6559	758	41
H(19F)	1679	7568	837	41
H(20D)	1108	5623	-358	63
H(20E)	1655	5760	-615	63
H(20F)	1117	6517	-604	63
H(21D)	3015	8471	-419	38
H(21E)	3355	8287	-73	38
H(21F)	2875	9131	-104	38
H(22B)	2943	6383	143	21
H(23B)	5078	4680	576	21
H(24D)	4076	4184	994	38
H(24E)	4728	3698	1017	38
H(24F)	4321	3550	691	38
H(25G)	5035	6182	851	36
H(25H)	5225	5356	1104	36
H(25I)	4550	5758	1107	36

	x	y	z	U(eq)
H(27B)	4735	3858	148	20
H(28B)	4366	3289	-365	21
H(30B)	3037	5262	-354	19

Table 10. Torsion angles [deg] for complex **3b**.

C(4A)-N(1A)-C(1A)-N(2A)	173.61(17)	C(22B)-Ru(1B)-O(1B)-C(26B)	8.36(12)
C(2A)-N(1A)-C(1A)-N(2A)	-2.3(2)	C(1B)-Ru(1B)-O(1B)-C(26B)	-86(3)
C(4A)-N(1A)-C(1A)-Ru(1A)	-15.4(3)	Cl(2B)-Ru(1B)-O(1B)-C(26B)	-91.53(11)
C(2A)-N(1A)-C(1A)-Ru(1A)	168.73(14)	Cl(1B)-Ru(1B)-O(1B)-C(26B)	109.36(11)
C(13A)-N(2A)-C(1A)-N(1A)	-166.93(17)	C(22B)-Ru(1B)-O(1B)-C(23B)	-165.51(15)
C(3A)-N(2A)-C(1A)-N(1A)	-1.5(2)	C(1B)-Ru(1B)-O(1B)-C(23B)	101(3)
C(13A)-N(2A)-C(1A)-Ru(1A)	23.3(3)	Cl(2B)-Ru(1B)-O(1B)-C(23B)	94.60(14)
C(3A)-N(2A)-C(1A)-Ru(1A)	-171.26(14)	Cl(1B)-Ru(1B)-O(1B)-C(23B)	-64.51(14)
C(22A)-Ru(1A)-C(1A)-N(1A)	170.61(15)	C(13B)-N(2B)-C(1B)-N(1B)	-179.05(18)
O(1A)-Ru(1A)-C(1A)-N(1A)	-75.4(9)	C(3B)-N(2B)-C(1B)-N(1B)	2.9(2)
Cl(2A)-Ru(1A)-C(1A)-N(1A)	70.71(15)	C(13B)-N(2B)-C(1B)-Ru(1B)	1.3(3)
Cl(1A)-Ru(1A)-C(1A)-N(1A)	-88.08(15)	C(3B)-N(2B)-C(1B)-Ru(1B)	-176.82(16)
C(22A)-Ru(1A)-C(1A)-N(2A)	-20.84(19)	C(4B)-N(1B)-C(1B)-N(2B)	-177.74(18)
O(1A)-Ru(1A)-C(1A)-N(2A)	93.1(9)	C(2B)-N(1B)-C(1B)-N(2B)	3.7(2)
Cl(2A)-Ru(1A)-C(1A)-N(2A)	-120.74(17)	C(4B)-N(1B)-C(1B)-Ru(1B)	2.0(3)
Cl(1A)-Ru(1A)-C(1A)-N(2A)	80.47(17)	C(2B)-N(1B)-C(1B)-Ru(1B)	-176.61(14)
C(1A)-N(1A)-C(2A)-C(3A)	4.8(2)	C(22B)-Ru(1B)-C(1B)-N(2B)	7.6(2)
C(4A)-N(1A)-C(2A)-C(3A)	-171.32(17)	O(1B)-Ru(1B)-C(1B)-N(2B)	101(2)
C(1A)-N(2A)-C(3A)-C(2A)	4.3(2)	Cl(2B)-Ru(1B)-C(1B)-N(2B)	107.16(19)
C(13A)-N(2A)-C(3A)-C(2A)	171.18(16)	Cl(1B)-Ru(1B)-C(1B)-N(2B)	-93.74(19)
N(1A)-C(2A)-C(3A)-N(2A)	-5.0(2)	C(22B)-Ru(1B)-C(1B)-N(1B)	-172.05(16)
C(1A)-N(1A)-C(4A)-C(9A)	97.7(2)	O(1B)-Ru(1B)-C(1B)-N(1B)	-78(3)
C(2A)-N(1A)-C(4A)-C(9A)	-86.7(2)	Cl(2B)-Ru(1B)-C(1B)-N(1B)	-72.49(15)
C(1A)-N(1A)-C(4A)-C(5A)	-86.7(2)	Cl(1B)-Ru(1B)-C(1B)-N(1B)	86.61(15)
C(2A)-N(1A)-C(4A)-C(5A)	88.9(2)	C(1B)-N(1B)-C(2B)-C(3B)	-8.1(2)
C(9A)-C(4A)-C(5A)-C(6A)	-5.9(3)	C(4B)-N(1B)-C(2B)-C(3B)	173.24(19)
N(1A)-C(4A)-C(5A)-C(6A)	178.53(18)	C(1B)-N(2B)-C(3B)-C(2B)	-7.7(2)
C(9A)-C(4A)-C(5A)-C(10A)	171.40(19)	C(13B)-N(2B)-C(3B)-C(2B)	174.11(18)
N(1A)-C(4A)-C(5A)-C(10A)	-4.2(3)	N(1B)-C(2B)-C(3B)-N(2B)	8.7(2)
C(4A)-C(5A)-C(6A)-C(7A)	2.1(3)	C(1B)-N(1B)-C(4B)-C(5B)	-85.8(2)
C(10A)-C(5A)-C(6A)-C(7A)	-175.3(2)	C(2B)-N(1B)-C(4B)-C(5B)	92.7(2)
C(5A)-C(6A)-C(7A)-C(8A)	1.4(3)	C(1B)-N(1B)-C(4B)-C(9B)	95.6(2)
C(5A)-C(6A)-C(7A)-C(11A)	179.6(2)	C(2B)-N(1B)-C(4B)-C(9B)	-85.9(2)
C(6A)-C(7A)-C(8A)-C(9A)	-1.2(3)	C(9B)-C(4B)-C(5B)-C(6B)	-8.5(3)
C(11A)-C(7A)-C(8A)-C(9A)	-179.4(2)	N(1B)-C(4B)-C(5B)-C(6B)	172.99(17)
C(7A)-C(8A)-C(9A)-C(4A)	-2.5(3)	C(9B)-C(4B)-C(5B)-C(10B)	167.46(19)
C(7A)-C(8A)-C(9A)-C(12A)	173.04(19)	N(1B)-C(4B)-C(5B)-C(10B)	-11.1(3)
C(5A)-C(4A)-C(9A)-C(8A)	6.1(3)	C(4B)-C(5B)-C(6B)-C(7B)	2.0(3)
N(1A)-C(4A)-C(9A)-C(8A)	-178.37(17)	C(10B)-C(5B)-C(6B)-C(7B)	-174.02(19)
C(5A)-C(4A)-C(9A)-C(12A)	-169.29(19)	C(5B)-C(6B)-C(7B)-C(8B)	4.5(3)
N(1A)-C(4A)-C(9A)-C(12A)	6.2(3)	C(5B)-C(6B)-C(7B)-C(11B)	-176.4(2)
C(1A)-N(2A)-C(13A)-C(14A)	74.5(2)	C(6B)-C(7B)-C(8B)-C(9B)	-4.9(3)
C(3A)-N(2A)-C(13A)-C(14A)	-90.4(2)	C(11B)-C(7B)-C(8B)-C(9B)	176.0(2)
C(1A)-N(2A)-C(13A)-C(18A)	-108.9(2)	C(7B)-C(8B)-C(9B)-C(4B)	-1.2(3)
C(3A)-N(2A)-C(13A)-C(18A)	86.2(2)	C(7B)-C(8B)-C(9B)-C(12B)	176.21(19)

C(18A)-C(13A)-C(14A)-C(15A)	1.7(3)
N(2A)-C(13A)-C(14A)-C(15A)	178.23(16)
C(18A)-C(13A)-C(14A)-C(19A)	178.90(17)
N(2A)-C(13A)-C(14A)-C(19A)	-4.6(3)
C(13A)-C(14A)-C(15A)-C(16A)	-0.7(3)
C(19A)-C(14A)-C(15A)-C(16A)	-177.94(18)
C(14A)-C(15A)-C(16A)-C(17A)	-0.7(3)
C(14A)-C(15A)-C(16A)-C(20A)	178.48(18)
C(15A)-C(16A)-C(17A)-C(18A)	1.1(3)
C(20A)-C(16A)-C(17A)-C(18A)	-178.01(19)
C(16A)-C(17A)-C(18A)-C(13A)	-0.2(3)
C(16A)-C(17A)-C(18A)-C(21A)	176.82(18)
C(14A)-C(13A)-C(18A)-C(17A)	-1.3(3)
N(2A)-C(13A)-C(18A)-C(17A)	-177.77(16)
C(14A)-C(13A)-C(18A)-C(21A)	-178.28(17)
N(2A)-C(13A)-C(18A)-C(21A)	5.2(3)
C(1A)-Ru(1A)-C(22A)-C(31A)	-179.03(14)
O(1A)-Ru(1A)-C(22A)-C(31A)	4.87(14)
Cl(2A)-Ru(1A)-C(22A)-C(31A)	-79.25(15)
Cl(1A)-Ru(1A)-C(22A)-C(31A)	89.76(15)
C(22A)-Ru(1A)-O(1A)-C(26A)	-4.71(13)
C(1A)-Ru(1A)-O(1A)-C(26A)	-119.4(9)
Cl(2A)-Ru(1A)-O(1A)-C(26A)	94.16(12)
Cl(1A)-Ru(1A)-O(1A)-C(26A)	-106.79(12)
C(22A)-Ru(1A)-O(1A)-C(23A)	165.41(18)
C(1A)-Ru(1A)-O(1A)-C(23A)	50.7(9)
Cl(2A)-Ru(1A)-O(1A)-C(23A)	-95.72(17)
Cl(1A)-Ru(1A)-O(1A)-C(23A)	63.33(17)
C(26A)-O(1A)-C(23A)-C(25A)	71.8(3)
Ru(1A)-O(1A)-C(23A)-C(25A)	-97.4(2)
C(26A)-O(1A)-C(23A)-C(24A)	-162.69(18)
Ru(1A)-O(1A)-C(23A)-C(24A)	28.1(3)
C(23A)-O(1A)-C(26A)-C(27A)	12.9(3)
Ru(1A)-O(1A)-C(26A)-C(27A)	-176.12(17)
C(23A)-O(1A)-C(26A)-C(31A)	-167.59(18)
Ru(1A)-O(1A)-C(26A)-C(31A)	3.3(2)
O(1A)-C(26A)-C(27A)-C(28A)	179.48(19)
C(31A)-C(26A)-C(27A)-C(28A)	0.1(3)
C(26A)-C(27A)-C(28A)-C(29A)	0.4(3)
C(27A)-C(28A)-C(29A)-C(30A)	-1.0(3)
C(27A)-C(28A)-C(29A)-N(3A)	178.63(18)
O(2A)-N(3A)-C(29A)-C(30A)	-4.3(3)
O(3A)-N(3A)-C(29A)-C(30A)	175.69(18)
O(2A)-N(3A)-C(29A)-C(28A)	176.00(18)
O(3A)-N(3A)-C(29A)-C(28A)	-4.0(3)
C(28A)-C(29A)-C(30A)-C(31A)	1.1(3)
N(3A)-C(29A)-C(30A)-C(31A)	-178.54(17)
C(29A)-C(30A)-C(31A)-C(26A)	-0.6(3)
C(29A)-C(30A)-C(31A)-C(22A)	179.70(18)
O(1A)-C(26A)-C(31A)-C(30A)	-179.46(17)
C(27A)-C(26A)-C(31A)-C(30A)	0.0(3)
O(1A)-C(26A)-C(31A)-C(22A)	0.2(3)
C(27A)-C(26A)-C(31A)-C(22A)	179.73(19)
Ru(1A)-C(22A)-C(31A)-C(30A)	174.87(15)
Ru(1A)-C(22A)-C(31A)-C(26A)	-4.8(2)
C(5B)-C(4B)-C(9B)-C(8B)	8.1(3)
N(1B)-C(4B)-C(9B)-C(8B)	-173.34(17)
C(5B)-C(4B)-C(9B)-C(12B)	-169.24(19)
N(1B)-C(4B)-C(9B)-C(12B)	9.3(3)
C(1B)-N(2B)-C(13B)-C(14B)	90.0(2)
C(3B)-N(2B)-C(13B)-C(14B)	-92.0(2)
C(1B)-N(2B)-C(13B)-C(18B)	-87.9(2)
C(3B)-N(2B)-C(13B)-C(18B)	90.1(2)
C(18B)-C(13B)-C(14B)-C(15B)	2.5(3)
N(2B)-C(13B)-C(14B)-C(15B)	-175.28(17)
C(18B)-C(13B)-C(14B)-C(19B)	-179.26(18)
N(2B)-C(13B)-C(14B)-C(19B)	2.9(3)
C(13B)-C(14B)-C(15B)-C(16B)	0.4(3)
C(19B)-C(14B)-C(15B)-C(16B)	-177.81(19)
C(14B)-C(15B)-C(16B)-C(17B)	-2.0(3)
C(14B)-C(15B)-C(16B)-C(20B)	178.9(2)
C(15B)-C(16B)-C(17B)-C(18B)	0.8(3)
C(20B)-C(16B)-C(17B)-C(18B)	179.9(2)
C(16B)-C(17B)-C(18B)-C(13B)	2.0(3)
C(16B)-C(17B)-C(18B)-C(21B)	178.82(19)
C(14B)-C(13B)-C(18B)-C(17B)	-3.7(3)
N(2B)-C(13B)-C(18B)-C(17B)	174.10(16)
C(14B)-C(13B)-C(18B)-C(21B)	179.49(18)
N(2B)-C(13B)-C(18B)-C(21B)	-2.7(3)
C(1B)-Ru(1B)-C(22B)-C(31B)	169.80(15)
O(1B)-Ru(1B)-C(22B)-C(31B)	-8.62(14)
Cl(2B)-Ru(1B)-C(22B)-C(31B)	74.50(15)
Cl(1B)-Ru(1B)-C(22B)-C(31B)	-94.09(15)
C(26B)-O(1B)-C(23B)-C(25B)	167.67(15)
Ru(1B)-O(1B)-C(23B)-C(25B)	-19.0(2)
C(26B)-O(1B)-C(23B)-C(24B)	-70.6(2)
Ru(1B)-O(1B)-C(23B)-C(24B)	102.74(16)
C(23B)-O(1B)-C(26B)-C(27B)	-12.5(3)
Ru(1B)-O(1B)-C(26B)-C(27B)	172.95(15)
C(23B)-O(1B)-C(26B)-C(31B)	168.57(15)
Ru(1B)-O(1B)-C(26B)-C(31B)	-5.98(18)
O(1B)-C(26B)-C(27B)-C(28B)	-178.50(17)
C(31B)-C(26B)-C(27B)-C(28B)	0.3(3)
C(26B)-C(27B)-C(28B)-C(29B)	0.2(3)
C(27B)-C(28B)-C(29B)-C(30B)	-1.1(3)
C(27B)-C(28B)-C(29B)-N(3B)	179.10(17)
O(2B)-N(3B)-C(29B)-C(28B)	176.36(18)
O(3B)-N(3B)-C(29B)-C(28B)	-2.8(3)
O(2B)-N(3B)-C(29B)-C(30B)	-3.4(3)
O(3B)-N(3B)-C(29B)-C(30B)	177.42(17)
C(28B)-C(29B)-C(30B)-C(31B)	1.4(3)
N(3B)-C(29B)-C(30B)-C(31B)	-178.82(16)
C(29B)-C(30B)-C(31B)-C(26B)	-0.8(3)
C(29B)-C(30B)-C(31B)-C(22B)	178.43(17)
O(1B)-C(26B)-C(31B)-C(30B)	178.92(16)
C(27B)-C(26B)-C(31B)-C(30B)	-0.1(3)
O(1B)-C(26B)-C(31B)-C(22B)	-0.3(2)
C(27B)-C(26B)-C(31B)-C(22B)	-179.29(17)
Ru(1B)-C(22B)-C(31B)-C(30B)	-170.63(14)
Ru(1B)-C(22B)-C(31B)-C(26B)	8.6(2)

9.5. X-ray data of complex 4a

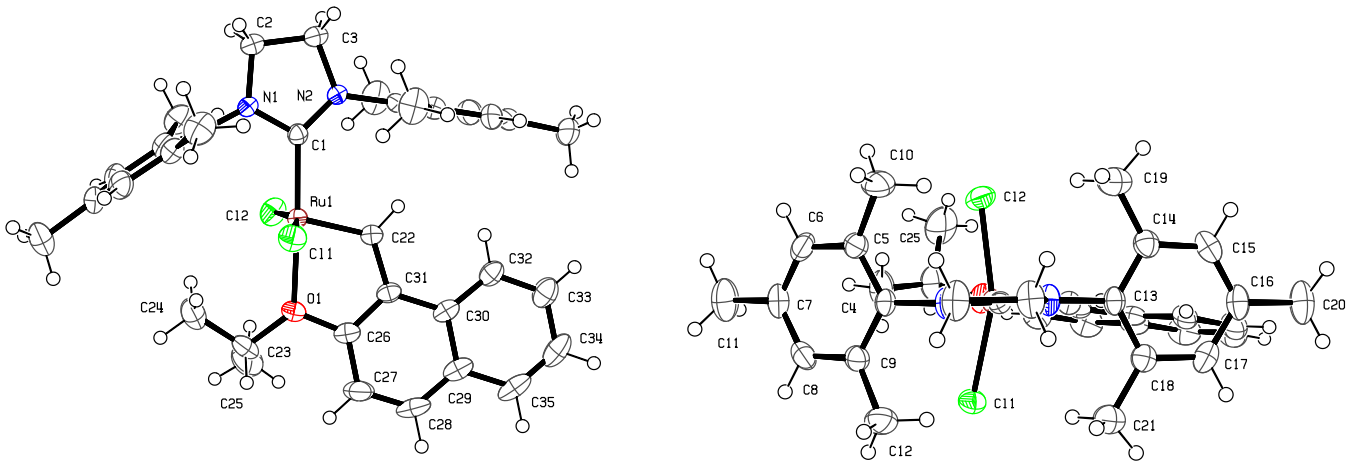


Figure 3. ORTEP[15] drawing (two orientations) of complex **4a** represented by thermal ellipsoids drawn at the 50% probability level.

Table 11. Crystal data and structure refinement for complex **4a**.

Identification code	4a
Empirical formula	C35 H40 Cl2 N2 O Ru
Formula weight	676.66
Temperature	230(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 12.2294(3) A alpha = 90 deg.
	b = 15.1477(3) A beta = 100.644(2) deg.
	c = 17.7310(4) A gamma = 90 deg.
Volume	3228.10(13) A^3
Z, Calculated density	4, 1.392 Mg/m^3
Absorption coefficient	0.681 mm^-1
F(000)	1400
Crystal size	0.40 x 0.27 x 0.19 mm
Theta range for data collection	2.69 to 28.72 deg.
Limiting indices	-16<=h<=15, -20<=k<=20, -23<=l<=23
Reflections collected / unique	52877 / 7984 [R(int) = 0.0179]
Completeness to theta = 28.00	99.3 \%
Absorption correction	Analytical
Max. and min. transmission	0.90 and 0.84
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7984 / 0 / 379

[15] We wish to acknowledge for use of a free version of Ortep-3 for Windows program: Farrugia, L. J. *J. Appl. Crystallogr.* **1997**, *30*, 565.

Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R1 = 0.0212, wR2 = 0.0583
R indices (all data)	R1 = 0.0314, wR2 = 0.0598
Extinction coefficient	0.0033(2)
Largest diff. peak and hole	0.322 and -0.335 e.A^-3

Table 12. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex **4a**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	**y**	**z**	**U(eq)**
Ru(1)	7019(1)	7933(1)	843(1)	24(1)
Cl(1)	5449(1)	7861(1)	-142(1)	38(1)
Cl(2)	8125(1)	8148(1)	2050(1)	42(1)
O(1)	6664(1)	9376(1)	790(1)	37(1)
N(1)	6675(1)	6142(1)	1308(1)	31(1)
N(2)	8058(1)	6105(1)	702(1)	30(1)
C(1)	7304(1)	6645(1)	922(1)	25(1)
C(2)	7001(2)	5208(1)	1369(1)	43(1)
C(3)	7959(1)	5181(1)	932(1)	40(1)
C(4)	5811(1)	6493(1)	1670(1)	27(1)
C(5)	6063(1)	6748(1)	2442(1)	33(1)
C(6)	5236(2)	7174(1)	2748(1)	40(1)
C(7)	4188(1)	7318(1)	2322(1)	41(1)
C(8)	3935(1)	6971(1)	1592(1)	39(1)
C(9)	4733(1)	6542(1)	1254(1)	32(1)
C(10)	7148(1)	6519(1)	2950(1)	48(1)
C(11)	3323(2)	7820(1)	2662(1)	66(1)
C(12)	4399(2)	6099(1)	487(1)	48(1)
C(13)	8880(1)	6322(1)	250(1)	27(1)
C(14)	9960(1)	6509(1)	626(1)	34(1)
C(15)	10736(1)	6729(1)	170(1)	41(1)
C(16)	10469(1)	6755(1)	-621(1)	38(1)
C(17)	9402(1)	6538(1)	-967(1)	39(1)
C(18)	8586(1)	6315(1)	-545(1)	32(1)
C(19)	10274(2)	6501(1)	1485(1)	56(1)
C(20)	11321(2)	7048(1)	-1089(1)	56(1)
C(21)	7423(2)	6099(1)	-943(1)	52(1)
C(22)	8012(1)	8318(1)	257(1)	28(1)
C(23)	6054(2)	9914(1)	1268(1)	49(1)
C(24)	5344(2)	9275(1)	1619(1)	59(1)
C(25)	6879(2)	10402(1)	1859(1)	71(1)
C(26)	7240(1)	9778(1)	286(1)	33(1)
C(27)	7078(2)	10659(1)	50(1)	46(1)
C(28)	7680(2)	10981(1)	-462(1)	50(1)
C(29)	8470(1)	10473(1)	-753(1)	39(1)
C(30)	8633(1)	9578(1)	-516(1)	30(1)
C(31)	7977(1)	9224(1)	10(1)	28(1)
C(32)	9424(1)	9077(1)	-820(1)	35(1)
C(33)	10004(1)	9434(1)	-1334(1)	45(1)
C(34)	9836(2)	10318(1)	-1569(1)	54(1)
C(35)	9097(2)	10819(1)	-1281(1)	52(1)

Table 13. Bond lengths [Å] and angles [deg] for complex **4a**.

Ru(1)-C(22)	1.8328(14)	C(15)-H(15)	0.9400
Ru(1)-C(1)	1.9821(14)	C(16)-C(17)	1.375(2)
Ru(1)-O(1)	2.2284(10)	C(16)-C(20)	1.514(2)
Ru(1)-Cl(2)	2.3326(4)	C(17)-C(18)	1.395(2)
Ru(1)-Cl(1)	2.3482(4)	C(17)-H(17)	0.9400
O(1)-C(26)	1.3768(17)	C(18)-C(21)	1.501(2)
O(1)-C(23)	1.4733(18)	C(19)-H(19A)	0.9700
N(1)-C(1)	1.3547(17)	C(19)-H(19B)	0.9700
N(1)-C(4)	1.4355(17)	C(19)-H(19C)	0.9700
N(1)-C(2)	1.4674(18)	C(20)-H(20A)	0.9700
N(2)-C(1)	1.3434(17)	C(20)-H(20B)	0.9700
N(2)-C(13)	1.4350(17)	C(20)-H(20C)	0.9700
N(2)-C(3)	1.4684(17)	C(21)-H(21A)	0.9700
C(2)-C(3)	1.520(2)	C(21)-H(21B)	0.9700
C(2)-H(2A)	0.9800	C(21)-H(21C)	0.9700
C(2)-H(2B)	0.9800	C(22)-C(31)	1.4395(18)
C(3)-H(3A)	0.9800	C(22)-H(22)	0.9400
C(3)-H(3B)	0.9800	C(23)-C(25)	1.508(3)
C(4)-C(9)	1.389(2)	C(23)-C(24)	1.510(2)
C(4)-C(5)	1.401(2)	C(23)-H(23)	0.9900
C(5)-C(6)	1.392(2)	C(24)-H(24A)	0.9700
C(5)-C(10)	1.500(2)	C(24)-H(24B)	0.9700
C(6)-C(7)	1.380(2)	C(24)-H(24C)	0.9700
C(6)-H(6)	0.9400	C(25)-H(25A)	0.9700
C(7)-C(8)	1.378(2)	C(25)-H(25B)	0.9700
C(7)-C(11)	1.516(2)	C(25)-H(25C)	0.9700
C(8)-C(9)	1.396(2)	C(26)-C(31)	1.386(2)
C(8)-H(8)	0.9400	C(26)-C(27)	1.402(2)
C(9)-C(12)	1.504(2)	C(27)-C(28)	1.361(2)
C(10)-H(10A)	0.9700	C(27)-H(27)	0.9400
C(10)-H(10B)	0.9700	C(28)-C(29)	1.406(2)
C(10)-H(10C)	0.9700	C(28)-H(28)	0.9400
C(11)-H(11A)	0.9700	C(29)-C(35)	1.416(2)
C(11)-H(11B)	0.9700	C(29)-C(30)	1.422(2)
C(11)-H(11C)	0.9700	C(30)-C(32)	1.412(2)
C(12)-H(12A)	0.9700	C(30)-C(31)	1.4414(19)
C(12)-H(12B)	0.9700	C(32)-C(33)	1.367(2)
C(12)-H(12C)	0.9700	C(32)-H(32)	0.9400
C(13)-C(18)	1.389(2)	C(33)-C(34)	1.405(2)
C(13)-C(14)	1.395(2)	C(33)-H(33)	0.9400
C(14)-C(15)	1.396(2)	C(34)-C(35)	1.351(3)
C(14)-C(19)	1.500(2)	C(34)-H(34)	0.9400
C(15)-C(16)	1.380(2)	C(35)-H(35)	0.9400
C(22)-Ru(1)-C(1)	103.12(6)	C(17)-C(16)-C(15)	118.30(14)
C(22)-Ru(1)-O(1)	78.93(5)	C(17)-C(16)-C(20)	121.17(16)
C(1)-Ru(1)-O(1)	177.89(5)	C(15)-C(16)-C(20)	120.49(16)
C(22)-Ru(1)-Cl(2)	98.22(5)	C(16)-C(17)-C(18)	122.15(15)
C(1)-Ru(1)-Cl(2)	90.50(4)	C(16)-C(17)-H(17)	118.9
O(1)-Ru(1)-Cl(2)	88.70(3)	C(18)-C(17)-H(17)	118.9
C(22)-Ru(1)-Cl(1)	97.45(5)	C(13)-C(18)-C(17)	117.71(14)
C(1)-Ru(1)-Cl(1)	96.63(4)	C(13)-C(18)-C(21)	121.57(14)
O(1)-Ru(1)-Cl(1)	83.54(3)	C(17)-C(18)-C(21)	120.70(15)

Cl(2)-Ru(1)-Cl(1)	160.835(16)	C(14)-C(19)-H(19A)	109.5
C(26)-O(1)-C(23)	120.18(12)	C(14)-C(19)-H(19B)	109.5
C(26)-O(1)-Ru(1)	110.01(8)	H(19A)-C(19)-H(19B)	109.5
C(23)-O(1)-Ru(1)	129.29(9)	C(14)-C(19)-H(19C)	109.5
C(1)-N(1)-C(4)	123.38(11)	H(19A)-C(19)-H(19C)	109.5
C(1)-N(1)-C(2)	114.05(12)	H(19B)-C(19)-H(19C)	109.5
C(4)-N(1)-C(2)	122.45(11)	C(16)-C(20)-H(20A)	109.5
C(1)-N(2)-C(13)	127.73(11)	C(16)-C(20)-H(20B)	109.5
C(1)-N(2)-C(3)	113.76(12)	H(20A)-C(20)-H(20B)	109.5
C(13)-N(2)-C(3)	118.43(11)	C(16)-C(20)-H(20C)	109.5
N(2)-C(1)-N(1)	106.77(12)	H(20A)-C(20)-H(20C)	109.5
N(2)-C(1)-Ru(1)	134.40(10)	H(20B)-C(20)-H(20C)	109.5
N(1)-C(1)-Ru(1)	118.73(10)	C(18)-C(21)-H(21A)	109.5
N(1)-C(2)-C(3)	102.27(11)	C(18)-C(21)-H(21B)	109.5
N(1)-C(2)-H(2A)	111.3	H(21A)-C(21)-H(21B)	109.5
C(3)-C(2)-H(2A)	111.3	C(18)-C(21)-H(21C)	109.5
N(1)-C(2)-H(2B)	111.3	H(21A)-C(21)-H(21C)	109.5
C(3)-C(2)-H(2B)	111.3	H(21B)-C(21)-H(21C)	109.5
H(2A)-C(2)-H(2B)	109.2	C(31)-C(22)-Ru(1)	119.38(11)
N(2)-C(3)-C(2)	103.12(12)	C(31)-C(22)-H(22)	120.3
N(2)-C(3)-H(3A)	111.1	Ru(1)-C(22)-H(22)	120.3
C(2)-C(3)-H(3A)	111.1	O(1)-C(23)-C(25)	109.04(15)
N(2)-C(3)-H(3B)	111.1	O(1)-C(23)-C(24)	105.91(13)
C(2)-C(3)-H(3B)	111.1	C(25)-C(23)-C(24)	112.89(17)
H(3A)-C(3)-H(3B)	109.1	O(1)-C(23)-H(23)	109.6
C(9)-C(4)-C(5)	121.30(13)	C(25)-C(23)-H(23)	109.6
C(9)-C(4)-N(1)	119.18(13)	C(24)-C(23)-H(23)	109.6
C(5)-C(4)-N(1)	119.47(13)	C(23)-C(24)-H(24A)	109.5
C(6)-C(5)-C(4)	117.69(14)	C(23)-C(24)-H(24B)	109.5
C(6)-C(5)-C(10)	119.92(15)	H(24A)-C(24)-H(24B)	109.5
C(4)-C(5)-C(10)	122.25(14)	C(23)-C(24)-H(24C)	109.5
C(7)-C(6)-C(5)	121.90(15)	H(24A)-C(24)-H(24C)	109.5
C(7)-C(6)-H(6)	119.0	H(24B)-C(24)-H(24C)	109.5
C(5)-C(6)-H(6)	119.0	C(23)-C(25)-H(25A)	109.5
C(8)-C(7)-C(6)	118.60(15)	C(23)-C(25)-H(25B)	109.5
C(8)-C(7)-C(11)	120.86(17)	H(25A)-C(25)-H(25B)	109.5
C(6)-C(7)-C(11)	120.51(17)	C(23)-C(25)-H(25C)	109.5
C(7)-C(8)-C(9)	121.78(15)	H(25A)-C(25)-H(25C)	109.5
C(7)-C(8)-H(8)	119.1	H(25B)-C(25)-H(25C)	109.5
C(9)-C(8)-H(8)	119.1	O(1)-C(26)-C(31)	113.93(12)
C(4)-C(9)-C(8)	117.90(14)	O(1)-C(26)-C(27)	123.58(14)
C(4)-C(9)-C(12)	121.90(14)	C(31)-C(26)-C(27)	122.46(15)
C(8)-C(9)-C(12)	120.06(14)	C(28)-C(27)-C(26)	118.41(16)
C(5)-C(10)-H(10A)	109.5	C(28)-C(27)-H(27)	120.8
C(5)-C(10)-H(10B)	109.5	C(26)-C(27)-H(27)	120.8
H(10A)-C(10)-H(10B)	109.5	C(27)-C(28)-C(29)	122.84(15)
C(5)-C(10)-H(10C)	109.5	C(27)-C(28)-H(28)	118.6
H(10A)-C(10)-H(10C)	109.5	C(29)-C(28)-H(28)	118.6
H(10B)-C(10)-H(10C)	109.5	C(28)-C(29)-C(35)	122.18(15)
C(7)-C(11)-H(11A)	109.5	C(28)-C(29)-C(30)	118.81(15)
C(7)-C(11)-H(11B)	109.5	C(35)-C(29)-C(30)	119.01(16)
H(11A)-C(11)-H(11B)	109.5	C(32)-C(30)-C(29)	117.92(14)
C(7)-C(11)-H(11C)	109.5	C(32)-C(30)-C(31)	123.29(13)
H(11A)-C(11)-H(11C)	109.5	C(29)-C(30)-C(31)	118.78(14)
H(11B)-C(11)-H(11C)	109.5	C(26)-C(31)-C(22)	117.05(13)

C(9)-C(12)-H(12A)	109.5	C(26)-C(31)-C(30)	118.65(13)
C(9)-C(12)-H(12B)	109.5	C(22)-C(31)-C(30)	124.27(13)
H(12A)-C(12)-H(12B)	109.5	C(33)-C(32)-C(30)	121.20(15)
C(9)-C(12)-H(12C)	109.5	C(33)-C(32)-H(32)	119.4
H(12A)-C(12)-H(12C)	109.5	C(30)-C(32)-H(32)	119.4
H(12B)-C(12)-H(12C)	109.5	C(32)-C(33)-C(34)	120.59(18)
C(18)-C(13)-C(14)	122.16(13)	C(32)-C(33)-H(33)	119.7
C(18)-C(13)-N(2)	119.20(13)	C(34)-C(33)-H(33)	119.7
C(14)-C(13)-N(2)	118.62(13)	C(35)-C(34)-C(33)	119.72(16)
C(13)-C(14)-C(15)	117.12(14)	C(35)-C(34)-H(34)	120.1
C(13)-C(14)-C(19)	121.73(14)	C(33)-C(34)-H(34)	120.1
C(15)-C(14)-C(19)	121.12(15)	C(34)-C(35)-C(29)	121.55(16)
C(16)-C(15)-C(14)	122.48(15)	C(34)-C(35)-H(35)	119.2
C(16)-C(15)-H(15)	118.8	C(29)-C(35)-H(35)	119.2
C(14)-C(15)-H(15)	118.8		

Table 14. Anisotropic displacement parameters ($A^2 \times 10^3$) for complex **4a**. The anisotropic displacement factor exponent takes the form: -2 $\pi^2 \times [h^2 \times a^2 \times U_{11} + ... + 2 \times h \times k \times a \times b \times U_{12}]$

	$\mathbf{U}_{11}$	$\mathbf{U}_{22}$	$\mathbf{U}_{33}$	$\mathbf{U}_{23}$	$\mathbf{U}_{13}$	$\mathbf{U}_{12}$
Ru(1)	27(1)	22(1)	24(1)	1(1)	6(1)	1(1)
Cl(1)	33(1)	42(1)	36(1)	4(1)	0(1)	3(1)
Cl(2)	50(1)	46(1)	28(1)	-2(1)	2(1)	-10(1)
O(1)	45(1)	24(1)	44(1)	-1(1)	17(1)	4(1)
N(1)	34(1)	23(1)	40(1)	6(1)	17(1)	1(1)
N(2)	34(1)	23(1)	38(1)	6(1)	16(1)	3(1)
C(1)	25(1)	28(1)	22(1)	2(1)	4(1)	1(1)
C(2)	52(1)	26(1)	58(1)	9(1)	27(1)	4(1)
C(3)	44(1)	25(1)	54(1)	8(1)	20(1)	4(1)
C(4)	29(1)	26(1)	30(1)	4(1)	12(1)	-1(1)
C(5)	32(1)	37(1)	30(1)	8(1)	6(1)	-4(1)
C(6)	48(1)	46(1)	28(1)	-2(1)	16(1)	-6(1)
C(7)	38(1)	41(1)	50(1)	4(1)	24(1)	0(1)
C(8)	25(1)	44(1)	47(1)	6(1)	7(1)	-3(1)
C(9)	31(1)	34(1)	32(1)	4(1)	6(1)	-6(1)
C(10)	45(1)	57(1)	38(1)	12(1)	-4(1)	-2(1)
C(11)	59(1)	65(1)	85(2)	-5(1)	42(1)	9(1)
C(12)	50(1)	51(1)	41(1)	-6(1)	2(1)	-15(1)
C(13)	28(1)	22(1)	34(1)	2(1)	13(1)	4(1)
C(14)	32(1)	33(1)	37(1)	3(1)	7(1)	4(1)
C(15)	27(1)	41(1)	56(1)	4(1)	10(1)	1(1)
C(16)	38(1)	31(1)	52(1)	6(1)	23(1)	7(1)
C(17)	50(1)	38(1)	33(1)	3(1)	18(1)	7(1)
C(18)	34(1)	29(1)	34(1)	1(1)	8(1)	3(1)
C(19)	48(1)	75(1)	42(1)	2(1)	-1(1)	-7(1)
C(20)	55(1)	48(1)	76(1)	15(1)	41(1)	7(1)
C(21)	44(1)	69(1)	42(1)	1(1)	3(1)	-8(1)
C(22)	29(1)	24(1)	29(1)	2(1)	5(1)	2(1)
C(23)	51(1)	35(1)	66(1)	-4(1)	26(1)	14(1)
C(24)	53(1)	58(1)	74(1)	-6(1)	33(1)	7(1)
C(25)	91(2)	52(1)	77(2)	-33(1)	35(1)	-7(1)

	$\mathbf{U}_{11}$	$\mathbf{U}_{22}$	$\mathbf{U}_{33}$	$\mathbf{U}_{23}$	$\mathbf{U}_{13}$	$\mathbf{U}_{12}$
C(26)	35(1)	25(1)	38(1)	3(1)	2(1)	0(1)
C(27)	51(1)	26(1)	60(1)	4(1)	9(1)	8(1)
C(28)	59(1)	24(1)	63(1)	15(1)	2(1)	1(1)
C(29)	42(1)	31(1)	41(1)	10(1)	-3(1)	-7(1)
C(30)	30(1)	28(1)	29(1)	5(1)	-4(1)	-7(1)
C(31)	29(1)	23(1)	29(1)	2(1)	-1(1)	-2(1)
C(32)	31(1)	37(1)	36(1)	7(1)	4(1)	-6(1)
C(33)	37(1)	53(1)	46(1)	8(1)	9(1)	-10(1)
C(34)	49(1)	63(1)	50(1)	20(1)	9(1)	-20(1)
C(35)	60(1)	40(1)	53(1)	22(1)	1(1)	-15(1)

Table 15. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($A^2 \times 10^3$) for complex **4a**.

	x	**y**	**z**	**U(eq)**
H(2A)	6389	4825	1131	52
H(2B)	7245	5033	1906	52
H(3A)	8645	4977	1260	48
H(3B)	7786	4794	482	48
H(6)	5396	7369	3260	47
H(8)	3205	7024	1314	46
H(10A)	7328	6963	3347	72
H(10B)	7731	6498	2646	72
H(10C)	7085	5947	3185	72
H(11A)	3570	7877	3212	99
H(11B)	2622	7503	2559	99
H(11C)	3223	8403	2432	99
H(12A)	4216	5486	563	72
H(12B)	5010	6128	209	72
H(12C)	3755	6396	195	72
H(15)	11468	6865	410	49
H(17)	9217	6540	-1506	47
H(19A)	9781	6890	1700	84
H(19B)	11036	6702	1638	84
H(19C)	10208	5906	1672	84
H(20A)	11319	7687	-1123	84
H(20B)	11136	6799	-1600	84
H(20C)	12053	6847	-843	84
H(21A)	7256	5489	-840	78
H(21B)	7362	6183	-1491	78
H(21C)	6901	6484	-753	78
H(22)	8539	7927	119	33
H(23)	5571	10342	940	59
H(24A)	4917	8912	1219	88
H(24B)	4841	9601	1879	88
H(24C)	5818	8900	1985	88
H(25A)	7401	9985	2142	106
H(25B)	6487	10706	2211	106
H(25C)	7278	10828	1605	106
H(27)	6565	11019	241	55

	x	y	z	U(eq)
H(28)	7563	11568	-629	60
H(32)	9553	8486	-666	42
H(33)	10521	9086	-1533	54
H(34)	10236	10558	-1924	65
H(35)	8998	11412	-1434	62

Table 16. Torsion angles [deg] for complex **4a**.

C(22)-Ru(1)-O(1)-C(26)	7.51(10)	N(2)-C(13)-C(14)-C(15)	-179.19(13)
C(1)-Ru(1)-O(1)-C(26)	174.0(13)	C(18)-C(13)-C(14)-C(19)	-179.02(15)
Cl(2)-Ru(1)-O(1)-C(26)	106.14(9)	N(2)-C(13)-C(14)-C(19)	-0.9(2)
Cl(1)-Ru(1)-O(1)-C(26)	-91.41(9)	C(13)-C(14)-C(15)-C(16)	-0.7(2)
C(22)-Ru(1)-O(1)-C(23)	-164.13(14)	C(19)-C(14)-C(15)-C(16)	-179.00(16)
C(1)-Ru(1)-O(1)-C(23)	2.3(14)	C(14)-C(15)-C(16)-C(17)	-1.3(3)
Cl(2)-Ru(1)-O(1)-C(23)	-65.50(13)	C(14)-C(15)-C(16)-C(20)	176.48(15)
Cl(1)-Ru(1)-O(1)-C(23)	96.95(13)	C(15)-C(16)-C(17)-C(18)	1.5(2)
C(13)-N(2)-C(1)-N(1)	177.26(13)	C(20)-C(16)-C(17)-C(18)	-176.28(14)
C(3)-N(2)-C(1)-N(1)	0.66(17)	C(14)-C(13)-C(18)-C(17)	-2.6(2)
C(13)-N(2)-C(1)-Ru(1)	-6.5(2)	N(2)-C(13)-C(18)-C(17)	179.36(13)
C(3)-N(2)-C(1)-Ru(1)	176.87(12)	C(14)-C(13)-C(18)-C(21)	179.05(14)
C(4)-N(1)-C(1)-N(2)	176.59(12)	N(2)-C(13)-C(18)-C(21)	1.0(2)
C(2)-N(1)-C(1)-N(2)	0.41(17)	C(16)-C(17)-C(18)-C(13)	0.4(2)
C(4)-N(1)-C(1)-Ru(1)	-0.32(18)	C(16)-C(17)-C(18)-C(21)	178.79(15)
C(2)-N(1)-C(1)-Ru(1)	-176.50(11)	C(1)-Ru(1)-C(22)-C(31)	173.88(11)
C(22)-Ru(1)-C(1)-N(2)	5.99(15)	O(1)-Ru(1)-C(22)-C(31)	-6.63(11)
O(1)-Ru(1)-C(1)-N(2)	-160.4(12)	Cl(2)-Ru(1)-C(22)-C(31)	-93.67(11)
Cl(2)-Ru(1)-C(1)-N(2)	-92.57(14)	Cl(1)-Ru(1)-C(22)-C(31)	75.25(11)
Cl(1)-Ru(1)-C(1)-N(2)	105.26(14)	C(26)-O(1)-C(23)-C(25)	-69.48(19)
C(22)-Ru(1)-C(1)-N(1)	-178.15(11)	Ru(1)-O(1)-C(23)-C(25)	101.43(16)
O(1)-Ru(1)-C(1)-N(1)	15.5(14)	C(26)-O(1)-C(23)-C(24)	168.77(14)
Cl(2)-Ru(1)-C(1)-N(1)	83.29(10)	Ru(1)-O(1)-C(23)-C(24)	-20.3(2)
Cl(1)-Ru(1)-C(1)-N(1)	-78.88(11)	C(23)-O(1)-C(26)-C(31)	165.68(14)
C(1)-N(1)-C(2)-C(3)	-1.22(18)	Ru(1)-O(1)-C(26)-C(31)	-6.83(15)
C(4)-N(1)-C(2)-C(3)	-177.44(13)	C(23)-O(1)-C(26)-C(27)	-16.3(2)
C(1)-N(2)-C(3)-C(2)	-1.38(17)	Ru(1)-O(1)-C(26)-C(27)	171.16(13)
C(13)-N(2)-C(3)-C(2)	-178.32(13)	O(1)-C(26)-C(27)-C(28)	-178.71(15)
N(1)-C(2)-C(3)-N(2)	1.43(16)	C(31)-C(26)-C(27)-C(28)	-0.9(3)
C(1)-N(1)-C(4)-C(9)	90.38(17)	C(26)-C(27)-C(28)-C(29)	-1.1(3)
C(2)-N(1)-C(4)-C(9)	-93.76(18)	C(27)-C(28)-C(29)-C(35)	-179.43(17)
C(1)-N(1)-C(4)-C(5)	-92.05(17)	C(27)-C(28)-C(29)-C(30)	1.4(3)
C(2)-N(1)-C(4)-C(5)	83.82(19)	C(28)-C(29)-C(30)-C(32)	179.49(14)
C(9)-C(4)-C(5)-C(6)	-9.4(2)	C(35)-C(29)-C(30)-C(32)	0.3(2)
N(1)-C(4)-C(5)-C(6)	173.12(13)	C(28)-C(29)-C(30)-C(31)	0.3(2)
C(9)-C(4)-C(5)-C(10)	166.15(14)	C(35)-C(29)-C(30)-C(31)	-178.89(14)
N(1)-C(4)-C(5)-C(10)	-11.4(2)	O(1)-C(26)-C(31)-C(22)	2.20(19)
C(4)-C(5)-C(6)-C(7)	2.3(2)	C(27)-C(26)-C(31)-C(22)	-175.83(15)
C(10)-C(5)-C(6)-C(7)	-173.37(15)	O(1)-C(26)-C(31)-C(30)	-179.45(12)
C(5)-C(6)-C(7)-C(8)	4.8(2)	C(27)-C(26)-C(31)-C(30)	2.5(2)
C(5)-C(6)-C(7)-C(11)	-177.22(16)	Ru(1)-C(22)-C(31)-C(26)	5.09(18)
C(6)-C(7)-C(8)-C(9)	-5.2(2)	Ru(1)-C(22)-C(31)-C(30)	-173.16(11)
C(11)-C(7)-C(8)-C(9)	176.89(15)	C(32)-C(30)-C(31)-C(26)	178.69(14)

C(5)-C(4)-C(9)-C(8)	9.1(2)
N(1)-C(4)-C(9)-C(8)	-173.41(13)
C(5)-C(4)-C(9)-C(12)	-166.73(14)
N(1)-C(4)-C(9)-C(12)	10.8(2)
C(7)-C(8)-C(9)-C(4)	-1.6(2)
C(7)-C(8)-C(9)-C(12)	174.22(15)
C(1)-N(2)-C(13)-C(18)	-84.79(18)
C(3)-N(2)-C(13)-C(18)	91.67(17)
C(1)-N(2)-C(13)-C(14)	97.05(18)
C(3)-N(2)-C(13)-C(14)	-86.48(17)
C(18)-C(13)-C(14)-C(15)	2.7(2)
C(29)-C(30)-C(31)-C(26)	-2.2(2)
C(32)-C(30)-C(31)-C(22)	-3.1(2)
C(29)-C(30)-C(31)-C(22)	176.03(14)
C(29)-C(30)-C(32)-C(33)	-0.9(2)
C(31)-C(30)-C(32)-C(33)	178.18(14)
C(30)-C(32)-C(33)-C(34)	0.7(2)
C(32)-C(33)-C(34)-C(35)	0.3(3)
C(33)-C(34)-C(35)-C(29)	-1.0(3)
C(28)-C(29)-C(35)-C(34)	-178.52(17)
C(30)-C(29)-C(35)-C(34)	0.7(3)

9.6. X-ray data of complex 4b

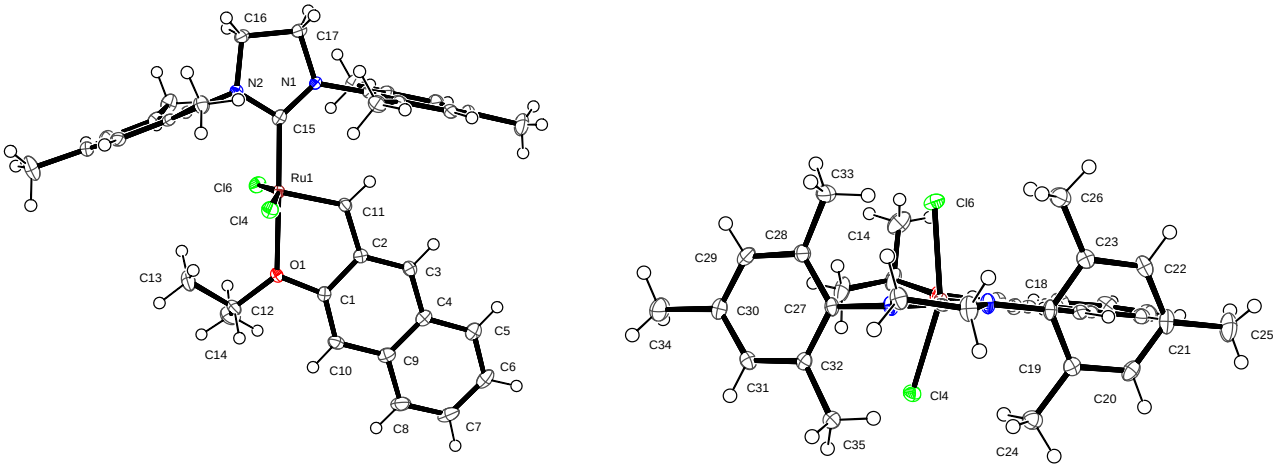


Figure 4. ORTEP drawing (two orientations) of complex **4b** represented by thermal ellipsoids drawn at the 50% probability level.

Table 17. Crystal data and structure refinement for complex **4b**.

Identification code	4b
Empirical formula	C35 H40 Cl2 N2 O Ru
Formula weight	676.66
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 11.7682(5) A alpha = 90.003(3) deg.
	b = 15.8365(5) A beta = 102.877(4) deg.
	c = 17.7410(7) A gamma = 90.003(3) deg.
Volume	3223.2(2) A^3
Z, Calculated density	4, 1.394 Mg/m^3
Absorption coefficient	0.682 mm^-1
F(000)	1400
Crystal size	0.32 x 0.12 x 0.05 mm
Theta range for data collection	2.61 to 27.50 deg.
Limiting indices	-15<=h<=15, -20<=k<=20, -23<=l<=23
Reflections collected / unique	59206 / 7389 [R(int) = 0.0403]
Completeness to theta = 27.50	99.9 %
Absorption correction	Analytical
Max. and min. transmission	0.97415 and 0.85102
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7389 / 0 / 530
Goodness-of-fit on F^2	0.917
Final R indices [I>2sigma(I)]	R1 = 0.0204, wR2 = 0.0449

R indices (all data)	R1 = 0.0350, wR2 = 0.0469
Largest diff. peak and hole	0.327 and -0.327 e.A^-3

Table 18. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex **4b**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ru(1)	3396(1)	7880(1)	3979(1)	12(1)
Cl(4)	5174(1)	7903(1)	4896(1)	18(1)
Cl(6)	2065(1)	8095(1)	2799(1)	20(1)
O(1)	3397(1)	9290(1)	4172(1)	17(1)
C(31)	6956(1)	7165(1)	3161(1)	15(1)
C(11)	2382(1)	7962(1)	4622(1)	14(1)
N(1)	2730(1)	6011(1)	3961(1)	14(1)
C(19)	2401(1)	6014(1)	5273(1)	15(1)
C(2)	2159(1)	8779(1)	4916(1)	14(1)
N(2)	4113(1)	6301(1)	3374(1)	14(1)
C(28)	4673(1)	7042(1)	2297(1)	16(1)
C(18)	1944(1)	6044(1)	4475(1)	14(1)
C(3)	1427(1)	8887(1)	5420(1)	15(1)
C(32)	6128(1)	6767(1)	3488(1)	13(1)
C(27)	4977(1)	6737(1)	3057(1)	13(1)
C(22)	11(1)	6155(1)	4671(1)	19(1)
C(16)	3854(2)	5406(1)	3175(1)	18(1)
C(10)	2540(1)	10291(1)	4936(1)	18(1)
C(4)	1217(1)	9691(1)	5697(1)	16(1)
C(7)	745(2)	11312(1)	6170(1)	26(1)
C(29)	5540(2)	7441(1)	2001(1)	18(1)
C(21)	432(1)	6146(1)	5468(1)	20(1)
C(35)	6513(2)	6337(1)	4262(1)	18(1)
C(23)	749(1)	6106(1)	4159(1)	16(1)
C(20)	1624(2)	6065(1)	5759(1)	18(1)
C(24)	3696(2)	5990(1)	5598(1)	20(1)
C(9)	1773(1)	10403(1)	5448(1)	18(1)
C(33)	3506(2)	6886(1)	1770(1)	22(1)
C(1)	2708(1)	9500(1)	4679(1)	15(1)
C(5)	450(1)	9818(1)	6204(1)	20(1)
C(17)	3050(2)	5177(1)	3707(1)	20(1)
C(6)	217(2)	10613(1)	6431(1)	23(1)
C(26)	286(2)	6151(1)	3298(1)	24(1)
C(8)	1514(2)	11216(1)	5698(1)	24(1)
C(30)	6676(1)	7512(1)	2421(1)	17(1)
C(34)	7593(2)	7917(2)	2067(1)	30(1)
C(25)	-390(2)	6230(2)	6006(1)	33(1)
C(12)	3870(2)	9961(1)	3761(1)	23(1)
C(13)	4810(2)	9550(1)	3424(1)	30(1)
C(14)	2909(2)	10345(1)	3151(1)	33(1)
C(15)	3396(1)	6645(1)	3791(1)	14(1)

Table 19. Bond lengths [Å] and angles [deg] for complex **4b**.

Ru(1)-C(11)	1.8310(15)	C(28)-C(33)	1.500(2)
Ru(1)-C(15)	1.9828(15)	C(18)-C(23)	1.397(2)

Ru(1)-O(1)	2.2593(11)	C(3)-C(4)	1.408(2)
Ru(1)-Cl(6)	2.3425(4)	C(32)-C(27)	1.401(2)
Ru(1)-Cl(4)	2.3470(4)	C(32)-C(35)	1.510(2)
O(1)-C(1)	1.3790(17)	C(22)-C(21)	1.390(2)
O(1)-C(12)	1.4681(18)	C(22)-C(23)	1.392(2)
C(31)-C(32)	1.391(2)	C(16)-C(17)	1.521(2)
C(31)-C(30)	1.392(2)	C(10)-C(1)	1.362(2)
C(11)-C(2)	1.441(2)	C(10)-C(9)	1.426(2)
N(1)-C(15)	1.3492(19)	C(4)-C(5)	1.422(2)
N(1)-C(18)	1.4369(18)	C(4)-C(9)	1.423(2)
N(1)-C(17)	1.4716(19)	C(7)-C(8)	1.371(2)
C(19)-C(20)	1.391(2)	C(7)-C(6)	1.398(3)
C(19)-C(18)	1.398(2)	C(29)-C(30)	1.382(2)
C(19)-C(24)	1.505(2)	C(21)-C(20)	1.389(2)
C(2)-C(3)	1.382(2)	C(21)-C(25)	1.509(2)
C(2)-C(1)	1.421(2)	C(23)-C(26)	1.506(2)
N(2)-C(15)	1.3546(18)	C(9)-C(8)	1.417(2)
N(2)-C(27)	1.4425(18)	C(5)-C(6)	1.369(2)
N(2)-C(16)	1.4753(19)	C(30)-C(34)	1.508(2)
C(28)-C(29)	1.398(2)	C(12)-C(14)	1.508(3)
C(28)-C(27)	1.402(2)	C(12)-C(13)	1.517(3)

C(11)-Ru(1)-C(15)	101.49(7)	C(32)-C(27)-C(28)	121.40(14)
C(11)-Ru(1)-O(1)	79.21(6)	C(32)-C(27)-N(2)	118.94(13)
C(15)-Ru(1)-O(1)	179.07(5)	C(28)-C(27)-N(2)	119.31(13)
C(11)-Ru(1)-Cl(6)	98.44(5)	C(21)-C(22)-C(23)	121.94(15)
C(15)-Ru(1)-Cl(6)	91.06(4)	N(2)-C(16)-C(17)	101.82(12)
O(1)-Ru(1)-Cl(6)	88.23(3)	C(1)-C(10)-C(9)	119.13(15)
C(11)-Ru(1)-Cl(4)	99.84(5)	C(3)-C(4)-C(5)	122.34(15)
C(15)-Ru(1)-Cl(4)	95.68(4)	C(3)-C(4)-C(9)	118.60(14)
O(1)-Ru(1)-Cl(4)	84.78(3)	C(5)-C(4)-C(9)	119.05(15)
Cl(6)-Ru(1)-Cl(4)	158.820(15)	C(8)-C(7)-C(6)	121.21(16)
C(1)-O(1)-C(12)	119.50(12)	C(30)-C(29)-C(28)	122.21(15)
C(1)-O(1)-Ru(1)	110.96(9)	C(20)-C(21)-C(22)	118.81(15)
C(12)-O(1)-Ru(1)	128.89(9)	C(20)-C(21)-C(25)	120.65(17)
C(32)-C(31)-C(30)	122.06(15)	C(22)-C(21)-C(25)	120.54(17)
C(2)-C(11)-Ru(1)	119.12(11)	C(22)-C(23)-C(18)	117.52(14)
C(15)-N(1)-C(18)	127.05(12)	C(22)-C(23)-C(26)	121.46(15)
C(15)-N(1)-C(17)	113.50(12)	C(18)-C(23)-C(26)	120.98(14)
C(18)-N(1)-C(17)	118.18(12)	C(21)-C(20)-C(19)	121.53(15)
C(20)-C(19)-C(18)	117.92(14)	C(8)-C(9)-C(4)	118.39(15)
C(20)-C(19)-C(24)	120.80(14)	C(8)-C(9)-C(10)	121.56(15)
C(18)-C(19)-C(24)	121.13(14)	C(4)-C(9)-C(10)	120.01(14)
C(3)-C(2)-C(1)	118.80(14)	C(10)-C(1)-O(1)	126.21(14)
C(3)-C(2)-C(11)	122.35(14)	C(10)-C(1)-C(2)	122.01(14)
C(1)-C(2)-C(11)	118.86(13)	O(1)-C(1)-C(2)	111.78(13)
C(15)-N(2)-C(27)	126.77(13)	C(6)-C(5)-C(4)	120.94(17)
C(15)-N(2)-C(16)	113.38(12)	N(1)-C(17)-C(16)	102.28(13)
C(27)-N(2)-C(16)	119.50(12)	C(5)-C(6)-C(7)	119.74(16)
C(29)-C(28)-C(27)	117.79(14)	C(7)-C(8)-C(9)	120.63(17)
C(29)-C(28)-C(33)	118.94(14)	C(29)-C(30)-C(31)	118.27(14)
C(27)-C(28)-C(33)	123.01(14)	C(29)-C(30)-C(34)	120.38(15)
C(23)-C(18)-C(19)	122.25(14)	C(31)-C(30)-C(34)	121.29(15)
C(23)-C(18)-N(1)	118.75(13)	O(1)-C(12)-C(14)	109.96(15)
C(19)-C(18)-N(1)	119.00(13)	O(1)-C(12)-C(13)	105.98(14)

C(2)-C(3)-C(4)	121.44(15)	C(14)-C(12)-C(13)	112.79(16)
C(31)-C(32)-C(27)	118.08(14)	N(1)-C(15)-N(2)	106.60(13)
C(31)-C(32)-C(35)	119.22(14)	N(1)-C(15)-Ru(1)	132.46(11)
C(27)-C(32)-C(35)	122.57(14)	N(2)-C(15)-Ru(1)	120.80(11)

Table 20. Anisotropic displacement parameters ($A^2 \times 10^3$) for complex **4b**. The anisotropic displacement factor exponent takes the form: -2 $\pi^2 \times [h^2 \times a^2 \times U_{11} + ... + 2 \times h \times k \times a \times b \times U_{12}]$

	$\mathbf{U}_{11}$	$\mathbf{U}_{22}$	$\mathbf{U}_{33}$	$\mathbf{U}_{23}$	$\mathbf{U}_{13}$	$\mathbf{U}_{12}$
Ru(1)	13(1)	12(1)	11(1)	0(1)	4(1)	-1(1)
Cl(4)	15(1)	21(1)	17(1)	-2(1)	2(1)	-2(1)
Cl(6)	24(1)	21(1)	14(1)	1(1)	1(1)	3(1)
O(1)	21(1)	13(1)	17(1)	2(1)	9(1)	-2(1)
C(31)	13(1)	14(1)	19(1)	-4(1)	4(1)	-2(1)
C(11)	15(1)	13(1)	15(1)	2(1)	4(1)	-1(1)
N(1)	15(1)	12(1)	17(1)	-3(1)	8(1)	-1(1)
C(19)	18(1)	8(1)	18(1)	1(1)	4(1)	-2(1)
C(2)	13(1)	14(1)	12(1)	1(1)	0(1)	1(1)
N(2)	14(1)	13(1)	17(1)	-3(1)	6(1)	-2(1)
C(28)	16(1)	17(1)	15(1)	-2(1)	4(1)	4(1)
C(18)	16(1)	10(1)	18(1)	-2(1)	9(1)	-3(1)
C(3)	14(1)	16(1)	15(1)	3(1)	2(1)	0(1)
C(32)	16(1)	11(1)	14(1)	-2(1)	6(1)	2(1)
C(27)	13(1)	12(1)	16(1)	-3(1)	7(1)	0(1)
C(22)	14(1)	19(1)	27(1)	-2(1)	7(1)	-2(1)
C(16)	18(1)	14(1)	23(1)	-4(1)	8(1)	0(1)
C(10)	19(1)	14(1)	20(1)	-1(1)	3(1)	-4(1)
C(4)	14(1)	20(1)	13(1)	-2(1)	-1(1)	3(1)
C(7)	22(1)	23(1)	31(1)	-14(1)	3(1)	3(1)
C(29)	25(1)	18(1)	13(1)	2(1)	7(1)	4(1)
C(21)	23(1)	16(1)	25(1)	-3(1)	15(1)	-3(1)
C(35)	17(1)	20(1)	17(1)	3(1)	4(1)	1(1)
C(23)	17(1)	14(1)	19(1)	-3(1)	4(1)	-1(1)
C(20)	27(1)	14(1)	15(1)	0(1)	7(1)	-3(1)
C(24)	20(1)	19(1)	21(1)	2(1)	3(1)	0(1)
C(9)	14(1)	19(1)	19(1)	-4(1)	-1(1)	0(1)
C(33)	18(1)	32(1)	16(1)	-2(1)	2(1)	3(1)
C(1)	13(1)	17(1)	13(1)	0(1)	3(1)	0(1)
C(5)	17(1)	24(1)	17(1)	-2(1)	2(1)	2(1)
C(17)	23(1)	14(1)	27(1)	-4(1)	12(1)	-1(1)
C(6)	17(1)	32(1)	20(1)	-9(1)	4(1)	5(1)
C(26)	19(1)	32(1)	21(1)	-3(1)	3(1)	1(1)
C(8)	24(1)	18(1)	31(1)	-9(1)	5(1)	-3(1)
C(30)	21(1)	15(1)	19(1)	-1(1)	10(1)	-2(1)
C(34)	28(1)	38(1)	27(1)	9(1)	10(1)	-9(1)
C(25)	32(1)	40(1)	33(1)	-4(1)	22(1)	-4(1)
C(12)	33(1)	17(1)	22(1)	-1(1)	14(1)	-10(1)
C(13)	36(1)	31(1)	29(1)	0(1)	20(1)	-10(1)
C(14)	50(1)	22(1)	28(1)	9(1)	11(1)	0(1)
C(15)	10(1)	19(1)	10(1)	-2(1)	-1(1)	1(1)

Table 21. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($A^2 \times 10^3$) for complex **4b**.

	x	y	z	U(eq)
H(17B)	3452(13)	4844(10)	4160(9)	14(4)
H(3)	1077(14)	8423(10)	5579(9)	15(4)
H(20)	1929(14)	6051(10)	6277(10)	17(4)
H(31)	7720(15)	7183(10)	3442(9)	17(4)
H(12)	4225(14)	10362(10)	4150(9)	18(4)
H(16A)	3457(14)	5373(10)	2637(9)	17(4)
H(33A)	3248(17)	7356(13)	1422(12)	42(6)
H(11)	1976(14)	7521(11)	4767(10)	20(5)
H(22)	-820(14)	6196(10)	4465(9)	17(4)
H(17A)	2385(15)	4872(11)	3436(10)	22(5)
H(6)	-285(14)	10673(10)	6747(9)	18(4)
H(10)	2886(14)	10760(11)	4782(9)	20(5)
H(35A)	6930(16)	5839(12)	4199(10)	30(5)
H(29)	5382(15)	7636(11)	1507(10)	21(5)
H(13A)	4490(15)	9153(12)	3027(10)	28(5)
H(24B)	3888(16)	5952(12)	6164(12)	37(5)
H(16B)	4573(15)	5094(11)	3284(10)	21(5)
H(33B)	2936(16)	6780(11)	2060(11)	29(5)
H(24A)	4030(14)	5509(11)	5400(10)	21(5)
H(7)	557(16)	11855(13)	6286(11)	35(5)
H(24C)	4045(15)	6507(12)	5470(10)	27(5)
H(35B)	5895(15)	6195(11)	4503(10)	23(5)
H(5)	97(14)	9350(10)	6364(9)	15(4)
H(26C)	554(17)	6634(13)	3087(11)	38(6)
H(13B)	5372(17)	9223(12)	3829(11)	37(6)
H(35C)	7033(16)	6700(12)	4646(10)	28(5)
H(34C)	7298(16)	8020(12)	1543(11)	30(5)
H(13C)	5193(17)	9990(12)	3188(11)	37(6)
H(33C)	3541(17)	6392(13)	1477(11)	40(6)
H(8)	1900(15)	11676(12)	5538(10)	26(5)
H(26A)	-530(20)	6179(13)	3158(12)	50(7)
H(34B)	7791(17)	8483(13)	2279(11)	36(6)
H(26B)	536(15)	5676(12)	3044(10)	30(5)
H(14C)	3249(18)	10766(14)	2861(12)	51(6)
H(34A)	8290(20)	7614(15)	2127(13)	58(7)
H(14B)	2327(18)	10592(13)	3361(11)	41(6)
H(14A)	2538(16)	9928(12)	2793(11)	31(5)
H(25A)	-1020(20)	5942(15)	5860(13)	61(8)
H(25B)	-710(30)	6740(20)	5968(18)	113(12)
H(25C)	-90(20)	6114(15)	6478(15)	65(8)

Table 22. Torsion angles [deg] for complex **4b**.

C(11)-Ru(1)-O(1)-C(1)	2.48(10)	C(25)-C(21)-C(20)-C(19)	-177.98(17)
C(15)-Ru(1)-O(1)-C(1)	142(3)	C(18)-C(19)-C(20)-C(21)	-0.2(2)
Cl(6)-Ru(1)-O(1)-C(1)	101.42(9)	C(24)-C(19)-C(20)-C(21)	175.48(15)
Cl(4)-Ru(1)-O(1)-C(1)	-98.59(9)	C(3)-C(4)-C(9)-C(8)	176.95(15)

C(11)-Ru(1)-O(1)-C(12)	-168.06(13)
C(15)-Ru(1)-O(1)-C(12)	-29(3)
Cl(6)-Ru(1)-O(1)-C(12)	-69.11(12)
Cl(4)-Ru(1)-O(1)-C(12)	90.87(12)
C(15)-Ru(1)-C(11)-C(2)	178.38(11)
O(1)-Ru(1)-C(11)-C(2)	-2.24(11)
Cl(6)-Ru(1)-C(11)-C(2)	-88.80(12)
Cl(4)-Ru(1)-C(11)-C(2)	80.46(12)
Ru(1)-C(11)-C(2)-C(3)	-178.28(12)
Ru(1)-C(11)-C(2)-C(1)	1.87(19)
C(20)-C(19)-C(18)-C(23)	-1.4(2)
C(24)-C(19)-C(18)-C(23)	-176.99(14)
C(20)-C(19)-C(18)-N(1)	178.67(13)
C(24)-C(19)-C(18)-N(1)	3.0(2)
C(15)-N(1)-C(18)-C(23)	102.52(18)
C(17)-N(1)-C(18)-C(23)	-91.20(18)
C(15)-N(1)-C(18)-C(19)	-77.5(2)
C(17)-N(1)-C(18)-C(19)	88.77(18)
C(1)-C(2)-C(3)-C(4)	0.2(2)
C(11)-C(2)-C(3)-C(4)	-179.67(14)
C(30)-C(31)-C(32)-C(27)	-1.4(2)
C(30)-C(31)-C(32)-C(35)	174.50(15)
C(31)-C(32)-C(27)-C(28)	4.6(2)
C(35)-C(32)-C(27)-C(28)	-171.21(14)
C(31)-C(32)-C(27)-N(2)	177.82(13)
C(35)-C(32)-C(27)-N(2)	2.0(2)
C(29)-C(28)-C(27)-C(32)	-5.1(2)
C(33)-C(28)-C(27)-C(32)	168.95(15)
C(29)-C(28)-C(27)-N(2)	-178.34(13)
C(33)-C(28)-C(27)-N(2)	-4.3(2)
C(15)-N(2)-C(27)-C(32)	93.60(18)
C(16)-N(2)-C(27)-C(32)	-93.63(17)
C(15)-N(2)-C(27)-C(28)	-93.04(18)
C(16)-N(2)-C(27)-C(28)	79.74(18)
C(15)-N(2)-C(16)-C(17)	-13.74(18)
C(27)-N(2)-C(16)-C(17)	172.56(14)
C(2)-C(3)-C(4)-C(5)	178.74(15)
C(2)-C(3)-C(4)-C(9)	0.1(2)
C(27)-C(28)-C(29)-C(30)	2.6(2)
C(33)-C(28)-C(29)-C(30)	-171.75(15)
C(23)-C(22)-C(21)-C(20)	-1.6(2)
C(23)-C(22)-C(21)-C(25)	178.01(17)
C(21)-C(22)-C(23)-C(18)	0.1(2)
C(21)-C(22)-C(23)-C(26)	-177.54(16)
C(19)-C(18)-C(23)-C(22)	1.4(2)
N(1)-C(18)-C(23)-C(22)	-178.64(13)
C(19)-C(18)-C(23)-C(26)	179.05(15)
N(1)-C(18)-C(23)-C(26)	-1.0(2)
C(22)-C(21)-C(20)-C(19)	1.6(2)
C(5)-C(4)-C(9)-C(8)	-1.7(2)
C(3)-C(4)-C(9)-C(10)	-0.9(2)
C(5)-C(4)-C(9)-C(10)	-179.58(14)
C(1)-C(10)-C(9)-C(8)	-176.39(15)
C(1)-C(10)-C(9)-C(4)	1.4(2)
C(9)-C(10)-C(1)-O(1)	178.51(14)
C(9)-C(10)-C(1)-C(2)	-1.1(2)
C(12)-O(1)-C(1)-C(10)	-10.2(2)
Ru(1)-O(1)-C(1)-C(10)	178.23(13)
C(12)-O(1)-C(1)-C(2)	169.45(13)
Ru(1)-O(1)-C(1)-C(2)	-2.10(14)
C(3)-C(2)-C(1)-C(10)	0.3(2)
C(11)-C(2)-C(1)-C(10)	-179.81(14)
C(3)-C(2)-C(1)-O(1)	-179.34(13)
C(11)-C(2)-C(1)-O(1)	0.51(19)
C(3)-C(4)-C(5)-C(6)	-176.56(16)
C(9)-C(4)-C(5)-C(6)	2.0(2)
C(15)-N(1)-C(17)-C(16)	-12.75(18)
C(18)-N(1)-C(17)-C(16)	179.16(13)
N(2)-C(16)-C(17)-N(1)	14.60(16)
C(4)-C(5)-C(6)-C(7)	-0.6(3)
C(8)-C(7)-C(6)-C(5)	-1.3(3)
C(6)-C(7)-C(8)-C(9)	1.6(3)
C(4)-C(9)-C(8)-C(7)	-0.1(2)
C(10)-C(9)-C(8)-C(7)	177.78(16)
C(28)-C(29)-C(30)-C(31)	0.4(2)
C(28)-C(29)-C(30)-C(34)	177.51(17)
C(32)-C(31)-C(30)-C(29)	-1.0(2)
C(32)-C(31)-C(30)-C(34)	-178.08(16)
C(1)-O(1)-C(12)-C(14)	-71.91(18)
Ru(1)-O(1)-C(12)-C(14)	97.93(15)
C(1)-O(1)-C(12)-C(13)	165.90(14)
Ru(1)-O(1)-C(12)-C(13)	-24.26(19)
C(18)-N(1)-C(15)-N(2)	171.42(13)
C(17)-N(1)-C(15)-N(2)	4.60(18)
C(18)-N(1)-C(15)-Ru(1)	-13.1(2)
C(17)-N(1)-C(15)-Ru(1)	-179.95(12)
C(27)-N(2)-C(15)-N(1)	179.46(13)
C(16)-N(2)-C(15)-N(1)	6.31(17)
C(27)-N(2)-C(15)-Ru(1)	3.4(2)
C(16)-N(2)-C(15)-Ru(1)	-169.78(11)
C(11)-Ru(1)-C(15)-N(1)	9.64(16)
O(1)-Ru(1)-C(15)-N(1)	-129(3)
Cl(6)-Ru(1)-C(15)-N(1)	-89.19(14)
Cl(4)-Ru(1)-C(15)-N(1)	110.91(14)
C(11)-Ru(1)-C(15)-N(2)	-175.43(12)
O(1)-Ru(1)-C(15)-N(2)	46(3)
Cl(6)-Ru(1)-C(15)-N(2)	85.73(11)
Cl(4)-Ru(1)-C(15)-N(2)	-74.16(12)

9.7. X-ray data of complex 4d

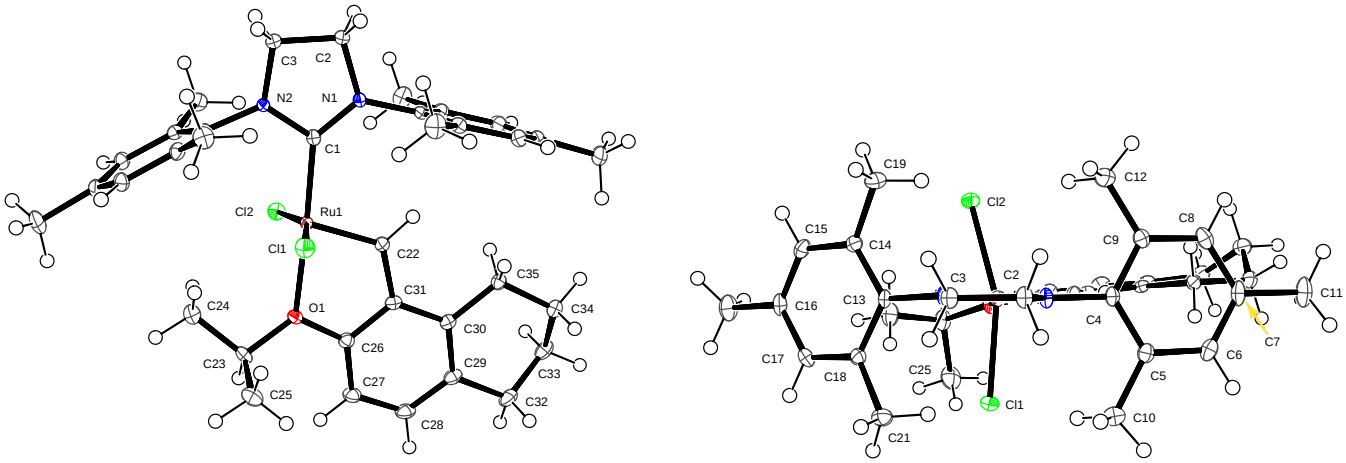


Figure 5. ORTEP drawing (two orientations) of complex **4d** represented by thermal ellipsoids drawn at the 50% probability level.

Table 23. Crystal data and structure refinement for complex **4d**.

Identification code	4d
Empirical formula	C35 H44 Cl2 N2 O Ru
Formula weight	680.69
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 12.4365(2) A alpha = 90 deg.
	b = 14.9182(3) A beta = 98.9540(10) deg.
	c = 17.4839(4) A gamma = 90 deg.
Volume	3204.26(11) A^3
Z, Calculated density	4, 1.411 Mg/m^3
Absorption coefficient	0.686 mm^-1
F(000)	1416
Crystal size	0.34 x 0.08 x 0.08 mm
Theta range for data collection	1.66 to 30.56 deg.
Limiting indices	-13<=h<=17, -14<=k<=21, -24<=l<=25
Reflections collected / unique	45786 / 9812 [R(int) = 0.0371]
Completeness to theta = 30.56	99.8 %
Absorption correction	Analytical
Max. and min. transmission	0.954 and 0.813
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9812 / 0 / 378
Goodness-of-fit on F^2	1.027

Final R indices [I>2sigma(I)]	R1 = 0.0276, wR2 = 0.0577
R indices (all data)	R1 = 0.0401, wR2 = 0.0620
Largest diff. peak and hole	0.482 and -0.645 e.A^-3

Table 24. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex **4d**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ru(1)	8003(1)	7043(1)	4280(1)	10(1)
Cl(1)	6917(1)	6778(1)	3087(1)	17(1)
Cl(2)	9552(1)	7151(1)	5231(1)	16(1)
O(1)	8345(1)	5584(1)	4349(1)	15(1)
N(1)	6979(1)	8904(1)	4393(1)	12(1)
N(2)	8381(1)	8853(1)	3796(1)	12(1)
C(1)	7735(1)	8347(1)	4183(1)	10(1)
C(2)	7094(1)	9838(1)	4155(1)	14(1)
C(3)	8056(1)	9796(1)	3708(1)	14(1)
C(4)	6153(1)	8692(1)	4847(1)	12(1)
C(5)	5104(1)	8496(1)	4471(1)	15(1)
C(6)	4317(1)	8288(1)	4926(1)	18(1)
C(7)	4552(1)	8269(1)	5729(1)	17(1)
C(8)	5593(1)	8496(1)	6083(1)	17(1)
C(9)	6406(1)	8712(1)	5652(1)	14(1)
C(10)	4836(1)	8497(1)	3601(1)	23(1)
C(11)	3697(1)	7981(1)	6205(1)	25(1)
C(12)	7540(1)	8942(1)	6047(1)	21(1)
C(13)	9232(1)	8486(1)	3425(1)	11(1)
C(14)	10296(1)	8463(1)	3830(1)	13(1)
C(15)	11089(1)	8036(1)	3482(1)	16(1)
C(16)	10853(1)	7655(1)	2752(1)	16(1)
C(17)	9817(1)	7764(1)	2337(1)	16(1)
C(18)	8999(1)	8197(1)	2656(1)	14(1)
C(19)	10599(1)	8931(1)	4595(1)	19(1)
C(20)	11709(1)	7156(1)	2402(1)	26(1)
C(21)	7933(1)	8399(1)	2153(1)	19(1)
C(22)	7028(1)	6679(1)	4905(1)	13(1)
C(23)	8978(1)	5038(1)	3877(1)	19(1)
C(24)	9686(1)	5685(1)	3517(1)	23(1)
C(25)	8218(2)	4520(1)	3276(1)	27(1)
C(26)	7747(1)	5170(1)	4846(1)	14(1)
C(27)	7845(1)	4279(1)	5060(1)	17(1)
C(28)	7179(1)	3965(1)	5567(1)	19(1)
C(29)	6419(1)	4503(1)	5856(1)	16(1)
C(30)	6326(1)	5404(1)	5641(1)	12(1)
C(31)	7016(1)	5749(1)	5137(1)	12(1)
C(32)	5726(1)	4107(1)	6412(1)	20(1)
C(33)	5367(1)	4814(1)	6938(1)	19(1)
C(34)	4781(1)	5559(1)	6443(1)	17(1)
C(35)	5529(1)	6022(1)	5949(1)	13(1)

Table 25. Bond lengths [Å] and angles [deg] for complex **4d**.

Ru(1)-C(22)	1.8359(15)	C(13)-C(18)	1.400(2)

Ru(1)-C(1)	1.9776(16)	C(13)-C(14)	1.4003(19)
Ru(1)-O(1)	2.2176(11)	C(14)-C(15)	1.390(2)
Ru(1)-Cl(1)	2.3351(4)	C(14)-C(19)	1.505(2)
Ru(1)-Cl(2)	2.3468(4)	C(15)-C(16)	1.387(2)
O(1)-C(26)	1.3740(19)	C(16)-C(17)	1.386(2)
O(1)-C(23)	1.4722(19)	C(16)-C(20)	1.505(2)
N(1)-C(1)	1.3479(19)	C(17)-C(18)	1.392(2)
N(1)-C(4)	1.4278(19)	C(18)-C(21)	1.503(2)
N(1)-C(2)	1.468(2)	C(22)-C(31)	1.447(2)
N(2)-C(1)	1.3574(19)	C(23)-C(24)	1.509(2)
N(2)-C(13)	1.4332(19)	C(23)-C(25)	1.511(2)
N(2)-C(3)	1.465(2)	C(26)-C(27)	1.382(2)
C(2)-C(3)	1.528(2)	C(26)-C(31)	1.406(2)
C(4)-C(9)	1.394(2)	C(27)-C(28)	1.386(2)
C(4)-C(5)	1.397(2)	C(28)-C(29)	1.393(2)
C(5)-C(6)	1.389(2)	C(29)-C(30)	1.396(2)
C(5)-C(10)	1.506(2)	C(29)-C(32)	1.516(2)
C(6)-C(7)	1.389(2)	C(30)-C(31)	1.417(2)
C(7)-C(8)	1.386(2)	C(30)-C(35)	1.513(2)
C(7)-C(11)	1.511(2)	C(32)-C(33)	1.512(3)
C(8)-C(9)	1.389(2)	C(33)-C(34)	1.522(2)
C(9)-C(12)	1.511(2)	C(34)-C(35)	1.529(2)

C(22)-Ru(1)-C(1)	102.91(7)	C(4)-C(9)-C(12)	120.96(14)
C(22)-Ru(1)-O(1)	79.44(6)	C(18)-C(13)-C(14)	121.03(14)
C(1)-Ru(1)-O(1)	177.61(5)	C(18)-C(13)-N(2)	119.69(13)
C(22)-Ru(1)-Cl(1)	97.94(5)	C(14)-C(13)-N(2)	119.20(13)
C(1)-Ru(1)-Cl(1)	91.35(4)	C(15)-C(14)-C(13)	118.00(14)
O(1)-Ru(1)-Cl(1)	87.86(3)	C(15)-C(14)-C(19)	120.32(13)
C(22)-Ru(1)-Cl(2)	98.26(5)	C(13)-C(14)-C(19)	121.56(14)
C(1)-Ru(1)-Cl(2)	95.85(4)	C(16)-C(15)-C(14)	121.84(14)
O(1)-Ru(1)-Cl(2)	84.20(3)	C(17)-C(16)-C(15)	118.65(15)
Cl(1)-Ru(1)-Cl(2)	160.316(15)	C(17)-C(16)-C(20)	120.26(15)
C(26)-O(1)-C(23)	119.71(13)	C(15)-C(16)-C(20)	121.06(15)
C(26)-O(1)-Ru(1)	110.91(9)	C(16)-C(17)-C(18)	121.53(15)
C(23)-O(1)-Ru(1)	128.82(10)	C(17)-C(18)-C(13)	118.21(13)
C(1)-N(1)-C(4)	127.40(13)	C(17)-C(18)-C(21)	119.53(14)
C(1)-N(1)-C(2)	113.84(13)	C(13)-C(18)-C(21)	122.10(14)
C(4)-N(1)-C(2)	118.65(12)	C(31)-C(22)-Ru(1)	119.14(11)
C(1)-N(2)-C(13)	123.30(13)	O(1)-C(23)-C(24)	106.11(14)
C(1)-N(2)-C(3)	114.28(12)	O(1)-C(23)-C(25)	110.03(13)
C(13)-N(2)-C(3)	122.06(12)	C(24)-C(23)-C(25)	112.31(15)
N(1)-C(1)-N(2)	106.58(13)	O(1)-C(26)-C(27)	124.71(15)
N(1)-C(1)-Ru(1)	134.31(11)	O(1)-C(26)-C(31)	113.44(14)
N(2)-C(1)-Ru(1)	119.03(11)	C(27)-C(26)-C(31)	121.85(15)
N(1)-C(2)-C(3)	103.02(12)	C(26)-C(27)-C(28)	117.49(16)
N(2)-C(3)-C(2)	102.18(12)	C(27)-C(28)-C(29)	122.98(16)
C(9)-C(4)-C(5)	121.79(14)	C(28)-C(29)-C(30)	119.33(15)
C(9)-C(4)-N(1)	119.18(13)	C(28)-C(29)-C(32)	119.55(15)
C(5)-C(4)-N(1)	119.00(13)	C(30)-C(29)-C(32)	121.10(15)
C(6)-C(5)-C(4)	117.83(14)	C(29)-C(30)-C(31)	118.92(15)
C(6)-C(5)-C(10)	120.93(14)	C(29)-C(30)-C(35)	121.47(14)
C(4)-C(5)-C(10)	121.23(14)	C(31)-C(30)-C(35)	119.59(14)
C(7)-C(6)-C(5)	121.81(14)	C(26)-C(31)-C(30)	119.38(14)
C(8)-C(7)-C(6)	118.73(15)	C(26)-C(31)-C(22)	116.85(14)

C(8)-C(7)-C(11)	120.84(16)	C(30)-C(31)-C(22)	123.76(14)
C(6)-C(7)-C(11)	120.41(15)	C(33)-C(32)-C(29)	111.68(14)
C(7)-C(8)-C(9)	121.49(15)	C(32)-C(33)-C(34)	108.88(14)
C(8)-C(9)-C(4)	118.28(14)	C(33)-C(34)-C(35)	111.82(13)
C(8)-C(9)-C(12)	120.74(14)	C(30)-C(35)-C(34)	114.56(14)

Table 26. Anisotropic displacement parameters ($A^2 \times 10^3$) for complex **4d**. The anisotropic displacement factor exponent takes the form: -2 $\pi^2 \times [h^2 \times a^2 \times U_{11} + ... + 2 \times h \times k \times a \times b \times U_{12}]$

	$\mathbf{U}_{11}$	$\mathbf{U}_{22}$	$\mathbf{U}_{33}$	$\mathbf{U}_{23}$	$\mathbf{U}_{13}$	$\mathbf{U}_{12}$
Ru(1)	10(1)	9(1)	9(1)	0(1)	2(1)	1(1)
Cl(1)	17(1)	20(1)	12(1)	-3(1)	0(1)	-1(1)
Cl(2)	14(1)	17(1)	14(1)	1(1)	-1(1)	1(1)
O(1)	17(1)	11(1)	18(1)	0(1)	7(1)	2(1)
N(1)	13(1)	11(1)	15(1)	2(1)	6(1)	2(1)
N(2)	12(1)	9(1)	16(1)	2(1)	7(1)	2(1)
C(1)	11(1)	14(1)	6(1)	-1(1)	0(1)	0(1)
C(2)	15(1)	11(1)	18(1)	2(1)	6(1)	2(1)
C(3)	16(1)	11(1)	17(1)	2(1)	5(1)	0(1)
C(4)	13(1)	9(1)	15(1)	1(1)	6(1)	2(1)
C(5)	14(1)	13(1)	18(1)	0(1)	4(1)	2(1)
C(6)	13(1)	15(1)	25(1)	1(1)	5(1)	1(1)
C(7)	17(1)	13(1)	25(1)	2(1)	12(1)	3(1)
C(8)	23(1)	14(1)	15(1)	2(1)	7(1)	4(1)
C(9)	16(1)	13(1)	15(1)	0(1)	4(1)	2(1)
C(10)	19(1)	30(1)	19(1)	-1(1)	0(1)	-1(1)
C(11)	24(1)	21(1)	36(1)	7(1)	19(1)	2(1)
C(12)	20(1)	27(1)	16(1)	1(1)	1(1)	-3(1)
C(13)	11(1)	11(1)	14(1)	2(1)	6(1)	1(1)
C(14)	13(1)	12(1)	13(1)	1(1)	1(1)	-1(1)
C(15)	10(1)	17(1)	21(1)	2(1)	3(1)	1(1)
C(16)	16(1)	16(1)	20(1)	4(1)	10(1)	2(1)
C(17)	19(1)	17(1)	12(1)	0(1)	6(1)	1(1)
C(18)	13(1)	16(1)	13(1)	2(1)	2(1)	0(1)
C(19)	19(1)	19(1)	18(1)	-4(1)	-1(1)	-3(1)
C(20)	22(1)	29(1)	31(1)	-3(1)	14(1)	7(1)
C(21)	17(1)	23(1)	16(1)	1(1)	-1(1)	2(1)
C(22)	12(1)	12(1)	13(1)	1(1)	3(1)	1(1)
C(23)	18(1)	15(1)	25(1)	-2(1)	9(1)	6(1)
C(24)	21(1)	21(1)	30(1)	0(1)	11(1)	2(1)
C(25)	33(1)	21(1)	30(1)	-11(1)	12(1)	-2(1)
C(26)	13(1)	13(1)	14(1)	-1(1)	2(1)	-1(1)
C(27)	18(1)	12(1)	21(1)	1(1)	2(1)	3(1)
C(28)	20(1)	11(1)	25(1)	4(1)	0(1)	1(1)
C(29)	15(1)	14(1)	17(1)	3(1)	-1(1)	-2(1)
C(30)	11(1)	13(1)	12(1)	1(1)	-2(1)	-1(1)
C(31)	12(1)	11(1)	13(1)	0(1)	-2(1)	-1(1)
C(32)	19(1)	16(1)	24(1)	7(1)	3(1)	-3(1)
C(33)	20(1)	21(1)	17(1)	6(1)	2(1)	-6(1)
C(34)	15(1)	18(1)	18(1)	1(1)	5(1)	-2(1)
C(35)	13(1)	14(1)	13(1)	2(1)	2(1)	0(1)

Table 27. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($A^2 \times 10^3$) for complex **4d**.

	x	y	z	U(eq)
H(2A)	7253	10239	4609	17
H(2B)	6427	10050	3819	17
H(3A)	7831	9955	3156	17
H(3B)	8652	10199	3938	17
H(6)	3599	8154	4682	21
H(8)	5754	8505	6632	20
H(10A)	4092	8277	3444	34
H(10B)	5348	8106	3385	34
H(10C)	4895	9109	3407	34
H(11A)	3682	7325	6233	38
H(11B)	2983	8201	5961	38
H(11C)	3871	8230	6728	38
H(12A)	7704	9567	5936	32
H(12B)	8067	8547	5854	32
H(12C)	7585	8861	6607	32
H(15)	11812	8005	3753	19
H(17)	9662	7538	1824	19
H(19A)	11231	8634	4894	29
H(19B)	9984	8906	4884	29
H(19C)	10778	9558	4506	29
H(20A)	11794	6552	2623	39
H(20B)	12403	7477	2514	39
H(20C)	11488	7114	1840	39
H(21A)	7977	8982	1903	29
H(21B)	7351	8413	2473	29
H(21C)	7774	7933	1757	29
H(22)	6538	7097	5074	15
H(23)	9448	4609	4218	22
H(24A)	9228	6066	3142	34
H(24B)	10197	5349	3252	34
H(24C)	10092	6061	3922	34
H(25A)	7792	4095	3534	40
H(25B)	8644	4191	2941	40
H(25C)	7725	4938	2962	40
H(27)	8350	3895	4866	21
H(28)	7244	3356	5726	23
H(32A)	5076	3819	6113	24
H(32B)	6147	3640	6730	24
H(33A)	6008	5061	7279	23
H(33B)	4872	4545	7267	23
H(34A)	4508	6007	6783	20
H(34B)	4146	5304	6100	20
H(35A)	5073	6318	5506	16
H(35B)	5944	6496	6263	16

Table 28. Torsion angles [deg] for complex **4d**.

C(22)-Ru(1)-O(1)-C(26)	-4.34(10)
Cl(1)-Ru(1)-O(1)-C(26)	-102.83(9)
Cl(2)-Ru(1)-O(1)-C(26)	95.20(9)
C(22)-Ru(1)-O(1)-C(23)	166.89(12)
Cl(1)-Ru(1)-O(1)-C(23)	68.40(11)
Cl(2)-Ru(1)-O(1)-C(23)	-93.57(11)
C(4)-N(1)-C(1)-N(2)	-176.57(13)
C(2)-N(1)-C(1)-N(2)	-0.50(16)
C(4)-N(1)-C(1)-Ru(1)	6.9(2)
C(2)-N(1)-C(1)-Ru(1)	-177.06(11)
C(13)-N(2)-C(1)-N(1)	-174.92(12)
C(3)-N(2)-C(1)-N(1)	-1.72(16)
C(13)-N(2)-C(1)-Ru(1)	2.27(18)
C(3)-N(2)-C(1)-Ru(1)	175.47(10)
C(22)-Ru(1)-C(1)-N(1)	-8.41(15)
Cl(1)-Ru(1)-C(1)-N(1)	90.06(14)
Cl(2)-Ru(1)-C(1)-N(1)	-108.29(14)
C(22)-Ru(1)-C(1)-N(2)	175.36(11)
Cl(1)-Ru(1)-C(1)-N(2)	-86.17(10)
Cl(2)-Ru(1)-C(1)-N(2)	75.48(11)
C(1)-N(1)-C(2)-C(3)	2.30(16)
C(4)-N(1)-C(2)-C(3)	178.74(12)
C(1)-N(2)-C(3)-C(2)	3.03(16)
C(13)-N(2)-C(3)-C(2)	176.33(13)
N(1)-C(2)-C(3)-N(2)	-2.94(14)
C(1)-N(1)-C(4)-C(9)	84.7(2)
C(2)-N(1)-C(4)-C(9)	-91.19(17)
C(1)-N(1)-C(4)-C(5)	-97.29(18)
C(2)-N(1)-C(4)-C(5)	86.81(18)
C(9)-C(4)-C(5)-C(6)	-2.3(2)
N(1)-C(4)-C(5)-C(6)	179.74(14)
C(9)-C(4)-C(5)-C(10)	178.55(16)
N(1)-C(4)-C(5)-C(10)	0.6(2)
C(4)-C(5)-C(6)-C(7)	-0.1(3)
C(10)-C(5)-C(6)-C(7)	178.98(17)
C(5)-C(6)-C(7)-C(8)	2.3(3)
C(5)-C(6)-C(7)-C(11)	-175.95(16)
C(6)-C(7)-C(8)-C(9)	-2.0(3)
C(11)-C(7)-C(8)-C(9)	176.18(16)
C(7)-C(8)-C(9)-C(4)	-0.3(2)
C(7)-C(8)-C(9)-C(12)	-178.92(16)
C(5)-C(4)-C(9)-C(8)	2.6(2)
N(1)-C(4)-C(9)-C(8)	-179.51(14)
C(5)-C(4)-C(9)-C(12)	-178.85(15)
N(1)-C(4)-C(9)-C(12)	-0.9(2)
C(1)-N(2)-C(13)-C(18)	88.89(18)
C(3)-N(2)-C(13)-C(18)	-83.79(19)
C(1)-N(2)-C(13)-C(14)	-94.09(18)
C(3)-N(2)-C(13)-C(14)	93.23(18)
C(18)-C(13)-C(14)-C(15)	-8.3(2)
N(2)-C(13)-C(14)-C(15)	174.73(14)
C(18)-C(13)-C(14)-C(19)	167.96(15)
N(2)-C(13)-C(14)-C(19)	-9.0(2)
C(13)-C(14)-C(15)-C(16)	1.1(2)
C(19)-C(14)-C(15)-C(16)	-175.18(16)
C(14)-C(15)-C(16)-C(17)	4.9(3)
C(14)-C(15)-C(16)-C(20)	-176.92(16)
C(15)-C(16)-C(17)-C(18)	-3.9(3)
C(20)-C(16)-C(17)-C(18)	177.86(16)
C(16)-C(17)-C(18)-C(13)	-3.0(2)
C(16)-C(17)-C(18)-C(21)	172.52(16)
C(14)-C(13)-C(18)-C(17)	9.2(2)
N(2)-C(13)-C(18)-C(17)	-173.83(14)
C(14)-C(13)-C(18)-C(21)	-166.16(15)
N(2)-C(13)-C(18)-C(21)	10.8(2)
C(1)-Ru(1)-C(22)-C(31)	-177.33(11)
O(1)-Ru(1)-C(22)-C(31)	3.14(11)
Cl(1)-Ru(1)-C(22)-C(31)	89.44(11)
Cl(2)-Ru(1)-C(22)-C(31)	-79.34(11)
C(26)-O(1)-C(23)-C(24)	-169.92(13)
Ru(1)-O(1)-C(23)-C(24)	19.52(17)
C(26)-O(1)-C(23)-C(25)	68.36(18)
Ru(1)-O(1)-C(23)-C(25)	-102.21(15)
C(23)-O(1)-C(26)-C(27)	13.3(2)
Ru(1)-O(1)-C(26)-C(27)	-174.56(12)
C(23)-O(1)-C(26)-C(31)	-167.58(12)
Ru(1)-O(1)-C(26)-C(31)	4.56(14)
O(1)-C(26)-C(27)-C(28)	-179.98(14)
C(31)-C(26)-C(27)-C(28)	1.0(2)
C(26)-C(27)-C(28)-C(29)	0.9(2)
C(27)-C(28)-C(29)-C(30)	-1.1(2)
C(27)-C(28)-C(29)-C(32)	-179.75(15)
C(28)-C(29)-C(30)-C(31)	-0.5(2)
C(32)-C(29)-C(30)-C(31)	178.11(13)
C(28)-C(29)-C(30)-C(35)	-178.83(14)
C(32)-C(29)-C(30)-C(35)	-0.2(2)
O(1)-C(26)-C(31)-C(30)	178.30(12)
C(27)-C(26)-C(31)-C(30)	-2.6(2)
O(1)-C(26)-C(31)-C(22)	-2.42(18)
C(27)-C(26)-C(31)-C(22)	176.72(14)
C(29)-C(30)-C(31)-C(26)	2.3(2)
C(35)-C(30)-C(31)-C(26)	-179.36(13)
C(29)-C(30)-C(31)-C(22)	-176.97(13)
C(35)-C(30)-C(31)-C(22)	1.4(2)
Ru(1)-C(22)-C(31)-C(26)	-1.64(18)
Ru(1)-C(22)-C(31)-C(30)	177.61(11)
C(28)-C(29)-C(32)-C(33)	153.16(14)
C(30)-C(29)-C(32)-C(33)	-25.4(2)
C(29)-C(32)-C(33)-C(34)	55.43(17)
C(32)-C(33)-C(34)-C(35)	-62.06(17)
C(29)-C(30)-C(35)-C(34)	-5.4(2)
C(31)-C(30)-C(35)-C(34)	176.25(13)
C(33)-C(34)-C(35)-C(30)	36.54(18)

9.8. X-ray data of complex 4e

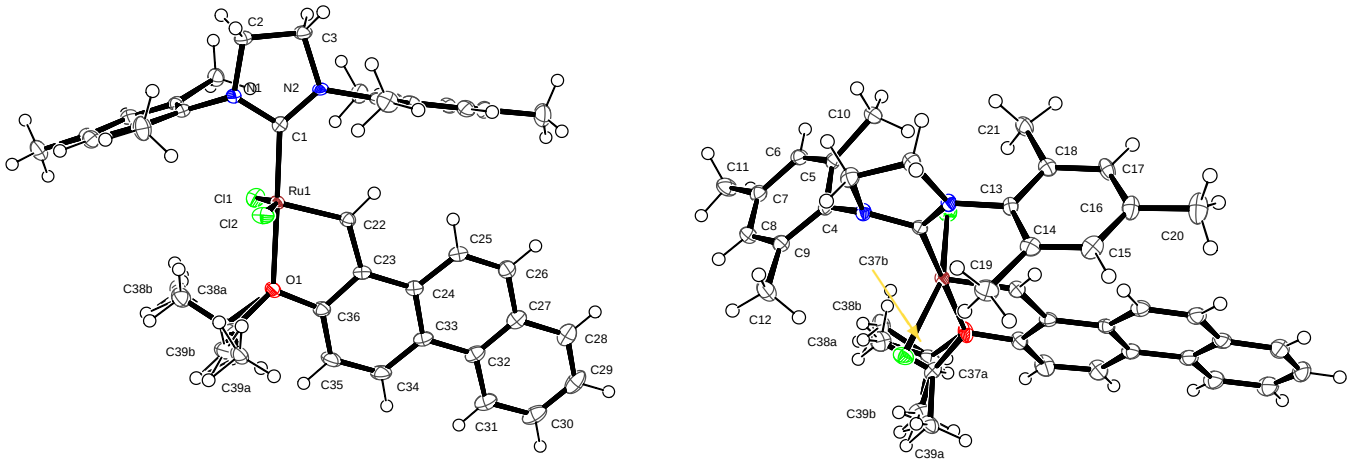


Figure 6. ORTEP drawing (two orientations) of complex **4e** represented by thermal ellipsoids drawn at the 50% probability level.

Table 29. Crystal data and structure refinement for complex **4e**.

Identification code	4e
Empirical formula	C39 H42 Cl2 N2 O Ru
Formula weight	726.72
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C2/c
Unit cell dimensions	a = 45.2974(18) A alpha = 90.0 deg.
	b = 11.2474(4) A beta = 103.075(2) deg.
	c = 13.6919(5) A gamma = 90.0 deg.
Volume	6794.9(4) A^3
Z, Calculated density	8, 1.421 Mg/m^3
Absorption coefficient	0.653 mm^-1
F(000)	3008
Crystal size	0.3 x 0.15 x 0.07 mm
Theta range for data collection	0.92 to 27.12 deg.
Limiting indices	-58<=h<=56, 0<=k<=14, 0<=l<=17
Reflections collected / unique	7486 / 7486 [R(int) = 0.0000]
Completeness to theta = 27.12	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.95 and 0.82
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7486 / 36 / 444
Goodness-of-fit on F^2	1.143
Final R indices [I>2sigma(I)]	R1 = 0.0363, wR2 = 0.0859
R indices (all data)	R1 = 0.0505, wR2 = 0.0911
Largest diff. peak and hole	0.706 and -0.795 e.A^-3

Table 30. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (A^2 x 10^3) for complex **4e**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	**y**	**z**	**U(eq)**
Ru(1)	-1085(1)	-12351(1)	-9975(1)	14(1)
Cl(1)	-810(1)	-12185(1)	-8326(1)	22(1)
Cl(2)	-1211(1)	-13070(1)	-11628(1)	20(1)
O(1)	-1265(1)	-14021(2)	-9426(2)	21(1)
N(1)	-650(1)	-10914(2)	-10719(2)	15(1)
N(2)	-1035(1)	-9782(2)	-10651(2)	14(1)
C(1)	-923(1)	-10888(2)	-10450(2)	13(1)
C(2)	-583(1)	-9794(2)	-11191(2)	19(1)
C(3)	-824(1)	-8960(2)	-10983(2)	19(1)
C(4)	-400(1)	-11672(2)	-10268(2)	16(1)
C(5)	-233(1)	-11386(2)	-9303(2)	16(1)
C(6)	7(1)	-12119(2)	-8858(2)	18(1)
C(7)	95(1)	-13079(2)	-9363(2)	19(1)
C(8)	-57(1)	-13277(2)	-10348(2)	21(1)
C(9)	-304(1)	-12585(2)	-10821(2)	18(1)
C(10)	-295(1)	-10264(2)	-8782(2)	21(1)
C(11)	355(1)	-13849(3)	-8837(2)	25(1)
C(12)	-453(1)	-12793(3)	-11909(2)	25(1)
C(13)	-1317(1)	-9302(2)	-10515(2)	14(1)
C(14)	-1561(1)	-9241(2)	-11336(2)	18(1)
C(15)	-1826(1)	-8705(3)	-11211(2)	22(1)
C(16)	-1848(1)	-8234(3)	-10291(2)	22(1)
C(17)	-1601(1)	-8311(2)	-9486(2)	18(1)
C(18)	-1328(1)	-8829(2)	-9576(2)	17(1)
C(19)	-1535(1)	-9766(3)	-12324(2)	24(1)
C(20)	-2138(1)	-7638(3)	-10176(3)	34(1)
C(21)	-1058(1)	-8877(3)	-8711(2)	21(1)
C(22)	-1460(1)	-11859(2)	-9828(2)	16(1)
C(23)	-1647(1)	-12662(2)	-9400(2)	16(1)
C(24)	-1930(1)	-12336(2)	-9177(2)	16(1)
C(25)	-2068(1)	-11203(2)	-9465(2)	18(1)
C(26)	-2337(1)	-10912(3)	-9265(2)	21(1)
C(27)	-2497(1)	-11700(3)	-8750(2)	21(1)
C(28)	-2781(1)	-11386(3)	-8559(2)	27(1)
C(29)	-2934(1)	-12151(3)	-8068(2)	31(1)
C(30)	-2806(1)	-13251(3)	-7750(2)	31(1)
C(31)	-2533(1)	-13588(3)	-7938(2)	26(1)
C(32)	-2371(1)	-12827(3)	-8450(2)	21(1)
C(33)	-2084(1)	-13158(3)	-8686(2)	19(1)
C(34)	-1956(1)	-14296(3)	-8470(2)	25(1)
C(35)	-1690(1)	-14631(3)	-8712(2)	26(1)
C(36)	-1536(1)	-13812(2)	-9175(2)	19(1)
C(37A)	-1199(4)	-15299(14)	-9624(14)	16(3)
C(38A)	-858(4)	-15230(14)	-9584(15)	26(3)
C(39A)	-1386(5)	-15785(13)	-10556(13)	21(3)
C(37B)	-1130(3)	-15224(8)	-9386(10)	17(2)
C(38B)	-797(3)	-15103(9)	-9286(11)	27(2)
C(39B)	-1290(4)	-15830(9)	-10361(9)	27(2)

Table 31. Bond lengths [Å] and angles [deg] for complex **4e**.

Ru(1)-C(22)	1.839(3)	C(14)-C(19)	1.504(4)
Ru(1)-C(1)	1.973(3)	C(15)-C(16)	1.390(4)
Ru(1)-O(1)	2.2435(19)	C(16)-C(17)	1.386(4)
Ru(1)-Cl(1)	2.3270(7)	C(16)-C(20)	1.512(4)
Ru(1)-Cl(2)	2.3496(7)	C(17)-C(18)	1.393(4)
O(1)-C(36)	1.369(3)	C(18)-C(21)	1.499(4)
O(1)-C(37B)	1.481(10)	C(22)-C(23)	1.448(4)
O(1)-C(37A)	1.504(17)	C(23)-C(36)	1.396(4)
N(1)-C(1)	1.369(3)	C(23)-C(24)	1.433(4)
N(1)-C(4)	1.439(3)	C(24)-C(33)	1.416(4)
N(1)-C(2)	1.478(3)	C(24)-C(25)	1.434(4)
N(2)-C(1)	1.348(3)	C(25)-C(26)	1.349(4)
N(2)-C(13)	1.435(3)	C(26)-C(27)	1.428(4)
N(2)-C(3)	1.475(3)	C(27)-C(28)	1.411(4)
C(2)-C(3)	1.514(4)	C(27)-C(32)	1.411(4)
C(4)-C(9)	1.401(4)	C(28)-C(29)	1.372(5)
C(4)-C(5)	1.404(4)	C(29)-C(30)	1.392(5)
C(5)-C(6)	1.389(4)	C(30)-C(31)	1.375(4)
C(5)-C(10)	1.508(4)	C(31)-C(32)	1.413(4)
C(6)-C(7)	1.388(4)	C(32)-C(33)	1.456(4)
C(7)-C(8)	1.387(4)	C(33)-C(34)	1.408(4)
C(7)-C(11)	1.505(4)	C(34)-C(35)	1.374(4)
C(8)-C(9)	1.397(4)	C(35)-C(36)	1.391(4)
C(9)-C(12)	1.507(4)	C(37A)-C(39A)	1.469(16)
C(13)-C(14)	1.388(4)	C(37A)-C(38A)	1.535(19)
C(13)-C(18)	1.403(4)	C(37B)-C(38B)	1.489(13)
C(14)-C(15)	1.389(4)	C(37B)-C(39B)	1.529(11)
C(22)-Ru(1)-C(1)	102.02(11)	C(13)-C(14)-C(19)	120.0(3)
C(22)-Ru(1)-O(1)	78.53(10)	C(15)-C(14)-C(19)	121.8(3)
C(1)-Ru(1)-O(1)	179.36(9)	C(14)-C(15)-C(16)	121.2(3)
C(22)-Ru(1)-Cl(1)	100.10(8)	C(17)-C(16)-C(15)	119.1(3)
C(1)-Ru(1)-Cl(1)	95.39(7)	C(17)-C(16)-C(20)	120.6(3)
O(1)-Ru(1)-Cl(1)	84.15(6)	C(15)-C(16)-C(20)	120.3(3)
C(22)-Ru(1)-Cl(2)	100.42(8)	C(16)-C(17)-C(18)	121.9(3)
C(1)-Ru(1)-Cl(2)	89.82(7)	C(17)-C(18)-C(13)	117.2(3)
O(1)-Ru(1)-Cl(2)	90.40(5)	C(17)-C(18)-C(21)	121.7(2)
Cl(1)-Ru(1)-Cl(2)	157.27(3)	C(13)-C(18)-C(21)	121.2(2)
C(36)-O(1)-C(37B)	122.3(5)	C(23)-C(22)-Ru(1)	119.6(2)
C(36)-O(1)-C(37A)	115.7(6)	C(36)-C(23)-C(24)	118.9(2)
C(36)-O(1)-Ru(1)	110.79(16)	C(36)-C(23)-C(22)	117.0(2)
C(37B)-O(1)-Ru(1)	126.8(4)	C(24)-C(23)-C(22)	124.1(2)
C(37A)-O(1)-Ru(1)	129.6(5)	C(33)-C(24)-C(23)	119.8(2)
C(1)-N(1)-C(4)	124.7(2)	C(33)-C(24)-C(25)	118.7(3)
C(1)-N(1)-C(2)	112.7(2)	C(23)-C(24)-C(25)	121.6(2)
C(4)-N(1)-C(2)	118.2(2)	C(26)-C(25)-C(24)	121.1(3)
C(1)-N(2)-C(13)	128.7(2)	C(25)-C(26)-C(27)	122.1(3)
C(1)-N(2)-C(3)	113.6(2)	C(28)-C(27)-C(32)	119.7(3)
C(13)-N(2)-C(3)	117.5(2)	C(28)-C(27)-C(26)	121.4(3)
N(2)-C(1)-N(1)	106.7(2)	C(32)-C(27)-C(26)	118.9(3)
N(2)-C(1)-Ru(1)	133.23(19)	C(29)-C(28)-C(27)	121.1(3)
N(1)-C(1)-Ru(1)	119.93(18)	C(28)-C(29)-C(30)	119.4(3)
N(1)-C(2)-C(3)	102.6(2)	C(31)-C(30)-C(29)	120.8(3)

N(2)-C(3)-C(2)	102.4(2)	C(30)-C(31)-C(32)	121.2(3)
C(9)-C(4)-C(5)	120.7(3)	C(27)-C(32)-C(31)	117.8(3)
C(9)-C(4)-N(1)	120.7(2)	C(27)-C(32)-C(33)	119.2(3)
C(5)-C(4)-N(1)	118.2(2)	C(31)-C(32)-C(33)	123.0(3)
C(6)-C(5)-C(4)	118.6(2)	C(34)-C(33)-C(24)	118.0(3)
C(6)-C(5)-C(10)	120.0(2)	C(34)-C(33)-C(32)	122.0(3)
C(4)-C(5)-C(10)	121.2(2)	C(24)-C(33)-C(32)	119.9(3)
C(7)-C(6)-C(5)	121.7(3)	C(35)-C(34)-C(33)	122.7(3)
C(8)-C(7)-C(6)	118.3(3)	C(34)-C(35)-C(36)	119.1(3)
C(8)-C(7)-C(11)	122.3(3)	O(1)-C(36)-C(35)	124.8(3)
C(6)-C(7)-C(11)	119.3(3)	O(1)-C(36)-C(23)	113.6(2)
C(7)-C(8)-C(9)	122.1(3)	C(35)-C(36)-C(23)	121.5(3)
C(8)-C(9)-C(4)	118.1(3)	C(39A)-C(37A)-O(1)	114.5(10)
C(8)-C(9)-C(12)	120.3(2)	C(39A)-C(37A)-C(38A)	115.4(11)
C(4)-C(9)-C(12)	121.6(3)	O(1)-C(37A)-C(38A)	100.5(10)
C(14)-C(13)-C(18)	122.4(2)	O(1)-C(37B)-C(38B)	108.7(7)
C(14)-C(13)-N(2)	118.7(2)	O(1)-C(37B)-C(39B)	105.4(7)
C(18)-C(13)-N(2)	118.7(2)	C(38B)-C(37B)-C(39B)	113.1(7)
C(13)-C(14)-C(15)	118.2(3)		

Table 32. Anisotropic displacement parameters ($A^2 \times 10^3$) for complex **4e**. The anisotropic displacement factor exponent takes the form: -2 $\pi^2 \times [h^2 \times a^2 \times U_{11} + ... + 2 \times h \times k \times a \times b \times U_{12}]$

	$\mathbf{U}_{11}$	$\mathbf{U}_{22}$	$\mathbf{U}_{33}$	$\mathbf{U}_{23}$	$\mathbf{U}_{13}$	$\mathbf{U}_{12}$
Ru(1)	17(1)	12(1)	13(1)	1(1)	6(1)	0(1)
Cl(1)	24(1)	28(1)	14(1)	2(1)	4(1)	0(1)
Cl(2)	28(1)	18(1)	17(1)	-2(1)	8(1)	-5(1)
O(1)	25(1)	14(1)	28(1)	3(1)	15(1)	3(1)
N(1)	16(1)	14(1)	18(1)	1(1)	6(1)	0(1)
N(2)	17(1)	12(1)	15(1)	2(1)	9(1)	-1(1)
C(1)	14(1)	17(1)	9(1)	-3(1)	2(1)	-1(1)
C(2)	21(2)	17(1)	22(1)	4(1)	9(1)	-2(1)
C(3)	24(2)	16(1)	20(1)	1(1)	12(1)	-3(1)
C(4)	15(1)	14(1)	19(1)	2(1)	7(1)	-2(1)
C(5)	18(1)	16(1)	19(1)	-1(1)	10(1)	-3(1)
C(6)	19(1)	19(1)	16(1)	-1(1)	5(1)	-4(1)
C(7)	18(1)	17(1)	23(1)	0(1)	6(1)	-2(1)
C(8)	22(2)	18(1)	24(2)	-5(1)	8(1)	-1(1)
C(9)	19(1)	18(1)	19(1)	-2(1)	7(1)	-4(1)
C(10)	21(2)	19(1)	22(1)	-6(1)	4(1)	0(1)
C(11)	27(2)	19(1)	29(2)	-4(1)	2(1)	5(1)
C(12)	27(2)	26(2)	22(2)	-5(1)	5(1)	7(1)
C(13)	16(1)	11(1)	17(1)	4(1)	8(1)	1(1)
C(14)	23(2)	13(1)	19(1)	3(1)	6(1)	-2(1)
C(15)	21(2)	21(1)	22(2)	9(1)	3(1)	1(1)
C(16)	20(2)	21(1)	27(2)	6(1)	11(1)	3(1)
C(17)	26(2)	15(1)	18(1)	3(1)	14(1)	4(1)
C(18)	22(2)	11(1)	19(1)	3(1)	8(1)	-1(1)
C(19)	27(2)	26(2)	17(1)	1(1)	1(1)	0(1)
C(20)	27(2)	35(2)	43(2)	8(2)	15(2)	11(2)
C(21)	23(2)	25(2)	16(1)	-5(1)	7(1)	1(1)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(22)	18(1)	14(1)	16(1)	2(1)	5(1)	0(1)
C(23)	19(1)	15(1)	13(1)	-1(1)	4(1)	-4(1)
C(24)	19(1)	16(1)	12(1)	-2(1)	4(1)	-3(1)
C(25)	20(2)	19(1)	16(1)	0(1)	4(1)	-5(1)
C(26)	19(2)	21(1)	20(1)	-2(1)	1(1)	-1(1)
C(27)	22(2)	27(2)	16(1)	-7(1)	4(1)	-5(1)
C(28)	22(2)	35(2)	23(2)	-8(1)	6(1)	-2(1)
C(29)	21(2)	48(2)	26(2)	-12(1)	12(1)	-6(2)
C(30)	29(2)	41(2)	27(2)	-8(1)	16(1)	-14(2)
C(31)	27(2)	30(2)	24(2)	-3(1)	10(1)	-9(1)
C(32)	21(2)	25(2)	18(1)	-5(1)	5(1)	-7(1)
C(33)	22(2)	20(1)	16(1)	-2(1)	7(1)	-7(1)
C(34)	32(2)	19(1)	29(2)	3(1)	16(1)	-6(1)
C(35)	35(2)	14(1)	33(2)	6(1)	16(1)	0(1)
C(36)	23(2)	17(1)	19(1)	1(1)	9(1)	-1(1)
C(37A)	15(5)	16(4)	16(5)	8(4)	2(4)	-1(3)
C(38A)	26(5)	22(4)	28(5)	3(4)	3(4)	3(3)
C(39A)	26(5)	14(4)	25(5)	-3(3)	8(4)	2(4)
C(37B)	24(4)	8(3)	19(4)	0(2)	1(3)	2(3)
C(38B)	28(4)	24(3)	31(4)	1(3)	9(3)	8(3)
C(39B)	30(4)	19(3)	32(4)	3(3)	5(3)	-3(3)

Table 33. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($A^2 \times 10^3$) for complex **4e**.

	x	y	z	U(eq)
H(2A)	-601	-9896	-11920	23
H(2B)	-377	-9502	-10880	23
H(3A)	-738	-8381	-10451	23
H(3B)	-926	-8523	-11595	23
H(6)	114	-11959	-8190	21
H(8)	10	-13903	-10712	25
H(10A)	-215	-10346	-8058	31
H(10B)	-515	-10128	-8915	31
H(10C)	-198	-9589	-9034	31
H(11A)	385	-14499	-9282	38
H(11B)	309	-14180	-8226	38
H(11C)	540	-13370	-8661	38
H(12A)	-666	-13006	-11969	37
H(12B)	-349	-13441	-12171	37
H(12C)	-441	-12066	-12293	37
H(15)	-1996	-8659	-11763	26
H(17)	-1617	-8002	-8855	22
H(19A)	-1733	-9734	-12796	36
H(19B)	-1468	-10595	-12224	36
H(19C)	-1387	-9311	-12594	36
H(20A)	-2176	-7837	-9518	51
H(20B)	-2307	-7918	-10704	51
H(20C)	-2118	-6775	-10230	51
H(21A)	-1107	-8486	-8128	32

	x	y	z	U(eq)
H(21B)	-887	-8469	-8892	32
H(21C)	-1004	-9709	-8546	32
H(22)	-1531	-11082	-10032	19
H(25)	-1968	-10648	-9802	22
H(26)	-2424	-10157	-9474	25
H(28)	-2867	-10634	-8773	32
H(29)	-3125	-11931	-7946	37
H(30)	-2910	-13776	-7399	37
H(31)	-2451	-14347	-7720	32
H(34)	-2058	-14855	-8143	30
H(35)	-1611	-15411	-8565	31
H(37A)	-1230	-15793	-9049	19
H(38A)	-825	-14782	-10164	39
H(38B)	-776	-16035	-9596	39
H(38C)	-755	-14829	-8966	39
H(39A)	-1599	-15801	-10509	32
H(39B)	-1319	-16595	-10657	32
H(39C)	-1366	-15284	-11122	32
H(37B)	-1170	-15672	-8799	21
H(38D)	-758	-14668	-9865	41
H(38E)	-704	-15895	-9258	41
H(38F)	-708	-14667	-8670	41
H(39D)	-1510	-15781	-10432	41
H(39E)	-1228	-16667	-10346	41
H(39F)	-1235	-15431	-10930	41

Table 34. Torsion angles [deg] for complex **4e**.

C(22)-Ru(1)-O(1)-C(36)	-5.80(18)	N(2)-C(13)-C(18)-C(17)	176.6(2)
Cl(1)-Ru(1)-O(1)-C(36)	95.77(17)	C(14)-C(13)-C(18)-C(21)	-178.2(3)
Cl(2)-Ru(1)-O(1)-C(36)	-106.35(17)	N(2)-C(13)-C(18)-C(21)	-3.2(4)
C(22)-Ru(1)-O(1)-C(37B)	170.4(7)	C(1)-Ru(1)-C(22)-C(23)	-174.6(2)
Cl(1)-Ru(1)-O(1)-C(37B)	-88.0(7)	O(1)-Ru(1)-C(22)-C(23)	5.0(2)
Cl(2)-Ru(1)-O(1)-C(37B)	69.9(7)	Cl(1)-Ru(1)-C(22)-C(23)	-76.9(2)
C(22)-Ru(1)-O(1)-C(37A)	150.7(10)	Cl(2)-Ru(1)-C(22)-C(23)	93.3(2)
Cl(1)-Ru(1)-O(1)-C(37A)	-107.7(10)	Ru(1)-C(22)-C(23)-C(36)	-3.8(3)
Cl(2)-Ru(1)-O(1)-C(37A)	50.2(10)	Ru(1)-C(22)-C(23)-C(24)	174.7(2)
C(13)-N(2)-C(1)-N(1)	179.3(2)	C(36)-C(23)-C(24)-C(33)	3.4(4)
C(3)-N(2)-C(1)-N(1)	-5.7(3)	C(22)-C(23)-C(24)-C(33)	-175.1(2)
C(13)-N(2)-C(1)-Ru(1)	4.1(4)	C(36)-C(23)-C(24)-C(25)	-174.8(2)
C(3)-N(2)-C(1)-Ru(1)	179.2(2)	C(22)-C(23)-C(24)-C(25)	6.8(4)
C(4)-N(1)-C(1)-N(2)	151.7(2)	C(33)-C(24)-C(25)-C(26)	0.8(4)
C(2)-N(1)-C(1)-N(2)	-4.1(3)	C(23)-C(24)-C(25)-C(26)	179.0(3)
C(4)-N(1)-C(1)-Ru(1)	-32.4(3)	C(24)-C(25)-C(26)-C(27)	0.8(4)
C(2)-N(1)-C(1)-Ru(1)	171.82(18)	C(25)-C(26)-C(27)-C(28)	-179.2(3)
C(22)-Ru(1)-C(1)-N(2)	-0.7(3)	C(25)-C(26)-C(27)-C(32)	-0.8(4)
Cl(1)-Ru(1)-C(1)-N(2)	-102.2(2)	C(32)-C(27)-C(28)-C(29)	1.2(4)
Cl(2)-Ru(1)-C(1)-N(2)	99.9(2)	C(26)-C(27)-C(28)-C(29)	179.6(3)
C(22)-Ru(1)-C(1)-N(1)	-175.3(2)	C(27)-C(28)-C(29)-C(30)	0.3(5)
Cl(1)-Ru(1)-C(1)-N(1)	83.11(19)	C(28)-C(29)-C(30)-C(31)	-1.2(5)
Cl(2)-Ru(1)-C(1)-N(1)	-74.73(19)	C(29)-C(30)-C(31)-C(32)	0.6(5)

C(1)-N(1)-C(2)-C(3)	11.5(3)
C(4)-N(1)-C(2)-C(3)	-146.0(2)
C(1)-N(2)-C(3)-C(2)	12.5(3)
C(13)-N(2)-C(3)-C(2)	-171.9(2)
N(1)-C(2)-C(3)-N(2)	-13.3(3)
C(1)-N(1)-C(4)-C(9)	113.2(3)
C(2)-N(1)-C(4)-C(9)	-92.2(3)
C(1)-N(1)-C(4)-C(5)	-74.1(3)
C(2)-N(1)-C(4)-C(5)	80.5(3)
C(9)-C(4)-C(5)-C(6)	-7.9(4)
N(1)-C(4)-C(5)-C(6)	179.4(2)
C(9)-C(4)-C(5)-C(10)	167.8(3)
N(1)-C(4)-C(5)-C(10)	-4.9(4)
C(4)-C(5)-C(6)-C(7)	3.7(4)
C(10)-C(5)-C(6)-C(7)	-172.1(3)
C(5)-C(6)-C(7)-C(8)	2.0(4)
C(5)-C(6)-C(7)-C(11)	-179.4(3)
C(6)-C(7)-C(8)-C(9)	-3.7(4)
C(11)-C(7)-C(8)-C(9)	177.8(3)
C(7)-C(8)-C(9)-C(4)	-0.5(4)
C(7)-C(8)-C(9)-C(12)	177.0(3)
C(5)-C(4)-C(9)-C(8)	6.4(4)
N(1)-C(4)-C(9)-C(8)	178.9(2)
C(5)-C(4)-C(9)-C(12)	-171.0(3)
N(1)-C(4)-C(9)-C(12)	1.5(4)
C(1)-N(2)-C(13)-C(14)	-98.7(3)
C(3)-N(2)-C(13)-C(14)	86.4(3)
C(1)-N(2)-C(13)-C(18)	86.1(3)
C(3)-N(2)-C(13)-C(18)	-88.8(3)
C(18)-C(13)-C(14)-C(15)	-1.0(4)
N(2)-C(13)-C(14)-C(15)	-175.9(2)
C(18)-C(13)-C(14)-C(19)	-179.9(2)
N(2)-C(13)-C(14)-C(19)	5.1(4)
C(13)-C(14)-C(15)-C(16)	0.3(4)
C(19)-C(14)-C(15)-C(16)	179.3(3)
C(14)-C(15)-C(16)-C(17)	-0.4(4)
C(14)-C(15)-C(16)-C(20)	179.1(3)
C(15)-C(16)-C(17)-C(18)	1.1(4)
C(20)-C(16)-C(17)-C(18)	-178.4(3)
C(16)-C(17)-C(18)-C(13)	-1.7(4)
C(16)-C(17)-C(18)-C(21)	178.1(3)
C(14)-C(13)-C(18)-C(17)	1.6(4)
C(28)-C(27)-C(32)-C(31)	-1.8(4)
C(26)-C(27)-C(32)-C(31)	179.8(3)
C(28)-C(27)-C(32)-C(33)	177.6(3)
C(26)-C(27)-C(32)-C(33)	-0.8(4)
C(30)-C(31)-C(32)-C(27)	0.9(4)
C(30)-C(31)-C(32)-C(33)	-178.5(3)
C(23)-C(24)-C(33)-C(34)	-2.5(4)
C(25)-C(24)-C(33)-C(34)	175.7(3)
C(23)-C(24)-C(33)-C(32)	179.4(2)
C(25)-C(24)-C(33)-C(32)	-2.4(4)
C(27)-C(32)-C(33)-C(34)	-175.6(3)
C(31)-C(32)-C(33)-C(34)	3.8(4)
C(27)-C(32)-C(33)-C(24)	2.4(4)
C(31)-C(32)-C(33)-C(24)	-178.2(3)
C(24)-C(33)-C(34)-C(35)	0.2(5)
C(32)-C(33)-C(34)-C(35)	178.3(3)
C(33)-C(34)-C(35)-C(36)	1.1(5)
C(37B)-O(1)-C(36)-C(35)	10.7(8)
C(37A)-O(1)-C(36)-C(35)	27.0(9)
Ru(1)-O(1)-C(36)-C(35)	-172.9(2)
C(37B)-O(1)-C(36)-C(23)	-171.1(7)
C(37A)-O(1)-C(36)-C(23)	-154.8(8)
Ru(1)-O(1)-C(36)-C(23)	5.3(3)
C(34)-C(35)-C(36)-O(1)	177.9(3)
C(34)-C(35)-C(36)-C(23)	-0.1(5)
C(24)-C(23)-C(36)-O(1)	179.7(2)
C(22)-C(23)-C(36)-O(1)	-1.8(4)
C(24)-C(23)-C(36)-C(35)	-2.1(4)
C(22)-C(23)-C(36)-C(35)	176.5(3)
C(36)-O(1)-C(37A)-C(39A)	70.6(12)
C(37B)-O(1)-C(37A)-C(39A)	-171(4)
Ru(1)-O(1)-C(37A)-C(39A)	-85.0(12)
C(36)-O(1)-C(37A)-C(38A)	-165.1(7)
C(37B)-O(1)-C(37A)-C(38A)	-46(3)
Ru(1)-O(1)-C(37A)-C(38A)	39.3(11)
C(36)-O(1)-C(37B)-C(38B)	-157.1(6)
C(37A)-O(1)-C(37B)-C(38B)	134(4)
Ru(1)-O(1)-C(37B)-C(38B)	27.1(9)
C(36)-O(1)-C(37B)-C(39B)	81.4(8)
C(37A)-O(1)-C(37B)-C(39B)	12(3)
Ru(1)-O(1)-C(37B)-C(39B)	-94.4(7)