Supplementary Information

Aminooxazolinate; a chiral amidinate analogue

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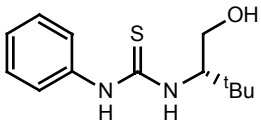
SYNTHESES

General comments. All manipulations of air-sensitive materials were carried out using standard Schlenk/glove box techniques under an atmosphere of dry argon. For organometallic preparations, hydrocarbon and ether solvents were pre-dried over sodium wire. These were then dried under reflux conditions over sodium for toluene, potassium for THF and benzene, sodium-potassium alloy for diethyl ether, petroleum ether and pentane, then distilled and degassed before use. Other solvents were dried under reflux conditions over the appropriate agents (calcium hydride for dichloromethane, pyridine and acetonitrile), then distilled and degassed before use. Deuterated solvents were degassed by the freeze-thaw method and dried over the appropriate agent (potassium for toluene, benzene and THF; calcium hydride for dichloromethane) before trap-to-trap distillation and storage in the glove box. All organic reagents were purchased from Aldrich Chemical Co. and used as received. NMR spectra were recorded on Bruker DPX-300, DPX-400, AC-400 and DPX-500 spectrometers and the spectra referenced internally using residual protio solvent resonances relative to tetramethylsilane (δ = 0.0 ppm). ATR-Infra-red spectra were carried out using Golden Gate apparatus or Nujol mulls on a Perkin Elmer FT-IR spectrometer. EI and CI mass spectra were obtained on a VG Autospec mass spectrometer. Elemental analyses were performed by Warwick Analytical Services.

(*S*)-1-hydroxy-2-(phenylthiourea)-3,3-dimethylbutane



To a stirred solution of (*S*)-*tert*-leucinol (0.10 g, 0.86 mmol) in THF (30 mL) was added phenylisothiocyanate (0.11 g, 0.78 mmol) dropwise *via* syringe. The reaction was left to stir overnight and the volatiles were removed *in vacuo* leaving a white solid. The product was washed with hexane (20 mL).

Yield = 0.17 g, 88%.

^{1}H NMR ($CDCl_3$): δ 7.65 (s, 1H, NH), 7.47 (t, *J* = 7 Hz, 1H, Ar-H), 7.22 - 7.37 (m, 4H, Ar-H), 6.16 (d, *J* = 8 Hz, 1H, NH), 4.55 (s, 1H, CH), 3.97 (m, 1H, CH_2), 3.67 (m, 1H, CH_2), 2.33 (s, 1H, OH), 0.93 (s, 9H, ^{t}Bu).

^{13}C NMR ($CDCl_3$): δ 166.9 (C=S), 143.8 (Ar), 130.7, 128.1, 125.8, 65.2 (CH), 63.8 (CH_2), 34.4 (^{t}Bu), 27.4.

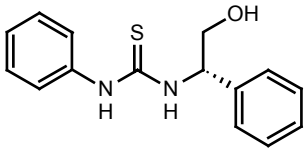
IR (neat) ν cm^{-1}: 3375, 3205, 2959, 1520, 1368, 1315, 1246, 1180, 1070, 1020.

MS (EI$^+$) m/z: 252 (M^+).

MS (CI$^+$) m/z: 270 (MNH_4^+).

EA for $C_{13}H_{20}ON_2S$, Calculated % C, 61.87; H, 7.99; N, 11.10. Found % C, 61.03; H, 7.82; N, 10.95.

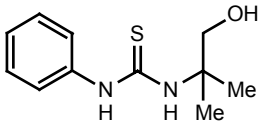
(*S*)-1-(2-hydroxy-1-phenylethyl)-3-phenylthiourea



To a stirred solution of amino-phenyl-methanol (2.25 g, 14.8 mmol) in THF (30 mL) was added phenylisothiocyanate (2.0 g, 14.8 mmol) dropwise *via* syringe. The reaction was left to stir overnight and the volatiles were removed *in vacuo* leaving a white solid. The product was washed with hexane (20 mL).

Yield 3.45 g, 85%
^{1}H NMR ($CDCl_3$): δ 7.85 (s, 1H, NH), 7.50-7.28 (m, 10H, Ar-H), 6.87 (d, *J* = 8 Hz, 1H, NH), 5.75 (s, 1H, OH), 4.04 (dd, 1H, CH_2), 3.96 (dd, 1H, CH_2), 1.92 (bs, 1H, CH).
^{13}C(^{1}H) NMR ($CDCl_3$): δ 180.6 (C=S), 130.2, 130.0, 128.0, 127.3, 126.7, 125.0 (Ar), 66.1 (CH_2), 60.2 (CH).
MS (EI$^+$) m/z: 272 [M^+]
Anal. Calc'd for $C_{15}H_{16}N_2OS$: C, 66.15; H, 5.92; N, 10.29. Found: C, 65.73; H, 5.93; N, 10.19.

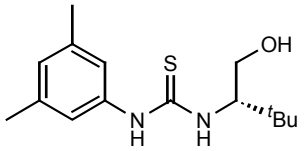
1-(2-hydroxy-1,1-dimethylethyl)-3-phenylthiourea



To a stirred solution of 2-amino-2-methyl-1-propanol (1.45 g, 16.3 mmol) in THF (30 mL) was added phenylisothiocyanate (2.0 g, 14.8 mmol) dropwise *via* syringe. The reaction was left to stir overnight and the volatiles were removed *in vacuo* leaving a white solid. The product was washed with hexane (20 mL).

Yield: 2.98 g, 90%
^{1}H NMR ($CDCl_3$): δ 7.40-7.32 (m, 4H, Ar-H), 7.23 (t, *J* = 7 Hz, 1H, *p*-Ar-H), 6.18 (s, 1H, NH), 3.71 (s, 2H, CH_2), 1.38 (s, 6H, Me). OH and NH not observed.
^{13}C(^{1}H) NMR ($CDCl_3$): δ 179.9 (C=S), 137.9, 130.0, 126.9, 124.9 (Ar), 70.0 (CMe_2), 58.2 (CH_2), 25.2 (CH_3).
MS (EI^+) m/z: 224 [M^+]
Anal. Calc'd for $C_{11}H_{16}N_2OS$: C, 58.90; H, 7.19; N, 12.49. Found: C, 58.87; H, 7.25; N, 12.56.

(*S*)-1-hydroxy-2-[(3,5-(dimethyl)phenylthiourea]-3,3-dimethylbutane



To a stirred solution of (*S*)-*tert*-leucinol (1.04 g, 8.89 mmol) in THF (30 mL) was added 3,5-dimethylphenylisothiocyanate (1.32 g, 8.08 mmol) dropwise *via* syringe. The reaction was left to stir overnight and the volatiles were removed *in vacuo* leaving a white solid. The product was washed with hexane (30 mL).

Yield = 1.83 g, 81 %.

^{1}H NMR ($CDCl_3$): δ 7.93 (s, 1H, NH), 6.85 (s, 1H, Ar-H), 6.78 (s, 2H, Ar-H), 6.21 (d, *J* = 7 Hz, 1H, NH), 4.46 (m, 1H, CH), 3.87 (dd, *J* = 8, 2 Hz, 1H, CH_2), 3.49 (dd, *J* = 8, 2 Hz, 1H, CH_2), 2.52 (s, 1H, OH), 2.25 (s, 6H, 2 x CH_3), 0.88 (s, 9H, ^{t}Bu).

^{13}C NMR ($CDCl_3$): δ 182.1 (C=S), 140.2 (Ar), 136.5, 129.6, 122.8, 65.1 (CH), 63.8 (CH_2), 34.5 (^{t}Bu), 27.4, 21.6 (CH_3).

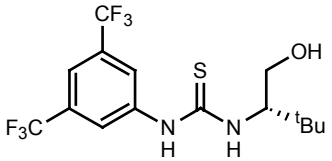
IR (neat) ν cm^{-1}: 3318, 3202, 2958, 1528, 1470, 1377, 1311, 1237, 1211, 1067.

MS (EI^+) m/z: 280 (M^+).

MS (CI^+) m/z: 281 (MH^+).

EA for $C_{15}H_{24}ON_2S$, Calculated % C, 64.24; H, 8.63; N, 9.99. Found % C, 64.16; H, 8.60; N, 9.88.

(*S*)-1-hydroxy-2-[3,5-bis(trifluoromethyl)phenylthiourea)]-3,3-dimethylbutane



To a stirred solution of (*S*)-*tert*-leucinol (0.48 g, 4.10 mmol) in THF (30 mL) was added 3,5-bis(triflouromethyl)phenylisothiocyanate (0.98 g, 3.63 mmol) dropwise *via* syringe. The reaction was left to stir overnight and the volatiles were removed *in vacuo* leaving a white solid. The product was washed with hexane (30 mL) and then recrystallised from a minimum amount of diethyl ether/hexane.

Yield = 1.21 g, 86 %.

^{1}H NMR ($CDCl_3$): δ 7.95 (s, 2H, Ar-H), 7.60 (s, 1H, Ar-H), 4.59 (s, 1H, NH), 3.99 (d, *J* = 7 Hz, 1H, NH), 3.70 (dd, *J* = 7, 2 Hz, 1H, CH_2), 3.59 (s, 1H, OH), 3.19 (t, *J* = 7 Hz, 1H, CH), 2.47 (dd, *J* = 7, 2 Hz, 1H, CH_2), 0.95 (s, 9H, ^{t}Bu).

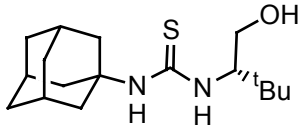
^{13}C NMR ($CDCl_3$): δ 179.8 (C=S), 123.1 (Ar), 122.4, 120.0, 117.8, 63.3 (CH), 61.6 (CH_2), 32.5 (^{t}Bu), 28.4 (CF_3), 25.8 (^{t}Bu).

IR (neat) ν cm^{-1}: 3258, 2966, 1537, 1472, 1381, 1274, 1170, 1124.

MS (EI$^+$) m/z: 388 (M^+).

EA for $C_{15}H_{18}ON_2SF_6$, Calculated % C, 46.39; H, 4.67; N, 7.21. Found % C, 46.18; H, 4.67; N, 7.01.

(*S*)-1-hydroxy-2-(1-adamantylthiourea)-3,3-dimethylbutane



To a stirred solution of (*S*)-*tert*-leucinol (1.00 g, 8.53 mmol) in THF (30 mL) was added 1-adamantylisothiocyanate (1.49 g, 7.76 mmol) dropwise *via* syringe. The reaction was left to stir overnight and the volatiles were removed *in vacuo* leaving a white solid. The product was washed with hexane (30 mL) and then recrystallised from a minimum amount of diethyl ether/hexane.

Yield = 1.95 g, 81 %.

^{1}H NMR ($CDCl_3$): δ 6.08 (s, 1H, NH), 5.93 (d, *J* = 7 Hz, 1H, CH), 4.34 (br, 1H, CH_2), 3.91 (dd, *J* = 7, 2 Hz, 1H, CH_2), 3.62 (dd, *J* = 7, 2 Hz, 1H, CH_2), 2.47 (s, 1H, OH), 2.08 - 2.11 (m, 3H, 3 x Ad-CH), 1.94 - 2.06 (m, 6H, 3 x Ad-CH_2), 1.58 - 1.70 (m, 6H, 3 x Ad-CH_2), 0.95 (s, 9H, ^{t}Bu).

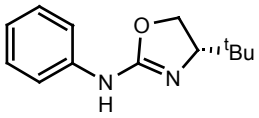
^{13}C NMR ($CDCl_3$): δ 183.8 (C=S), 70.1 (CH), 63.8 (CH_2), 54.4 (Ad-C), 42.8 (Ad-CH_2), 36.5 (Ad-CH_2), 34.5 (^{t}Bu), 29.8 (Ad-CH), 27.7 (^{t}Bu).

IR (neat) ν cm^{-1}: 3318, 3146, 2903, 1547, 1475, 1369, 1256, 1296, 1090, 1049, 692.

MS (EI$^+$) m/z: 310 (M^+).

EA for $C_{17}H_{30}ON_2S$, Calculated % C, 65.76; H, 9.74; N, 9.02. Found % C, 65.31; H, 9.46; N, 8.83.

(*S*)-2-phenylamino-4-*tert*-butyloxazoline HL[1]



A mixture of two solutions, one of NaOH (0.80 g, 20.0 mmol) in water (2 mL), and a second of TsCl (1.68 g, 8.81 mmol) in THF (5 mL) was added dropwise *via* syringe over 5 minutes to a stirred solution of 1-hydroxy-2-(phenylthiourea)-3,3-dimethylbutyl (2.02 g, 8.00 mmol) in THF (25 mL). After stirring overnight, water (20 mL) was added and the resultant suspension was extracted with Et_2O (3 x 20 mL). The combined organic layers were dried over magnesium sulphate, filtered and the solvent was removed *in vacuo*. The product was washed with hexane.

Yield = 1.27 g, 73%.

^{1}H NMR ($CDCl_3$): δ 7.25 - 7.35 (m, 4H, Ar-H), 6.97 - 7.02 (m, 1H, Ar-H), 4.31 (t, *J* = 8 Hz, 1H, CH_2), 4.19 (t, *J* = 8 Hz, 1H, CH_2), 3.76 - 3.79 (m, 1H, CH), 0.95 (s, 9H, ^{t}Bu). NH not observed.

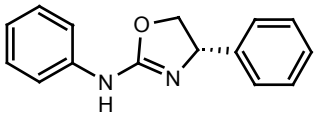
^{13}C NMR ($CDCl_3$): δ 154.2 (NHC(O)=N), 136.1 (Ar) 129.2, 122.5, 120.3, 71.8 (CH), 68.9 (CH_2), 34.3 (^{t}Bu), 25.8.

IR (neat) ν cm^{-1}: 2961, 2868, 1668, 1588, 1481, 1404, 1320, 1216, 1023.

MS (EI^+) m/z: 218 (M^+).

EA for $C_{13}H_{18}ON_2$, Calculated % C, 71.53; H, 8.31; N, 12.83. Found % C, 71.09; H, 8.20; N, 12.76.

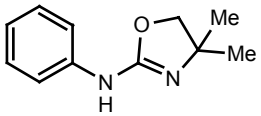
Synthesis of (*S*)-2-phenylamino-4-phenyloxazoline HL[2]



A mixture of two solutions, one of NaOH (1.10 g, 27.5 mmol) in water (2 mL), and a second of TsCl (2.30 g, 12.1 mmol) in THF (5 mL) was added dropwise *via* syringe over 5 minutes to a stirred solution of (*S*)-1-(2-hydroxy-1-phenylethyl)-3-phenylthiourea (3.00 g, 11.0 mmol) in THF (30 mL). After stirring overnight, water (20 mL) was added and the resultant suspension was extracted with Et_2O (3 x 20 mL). The combined organic layers were dried over magnesium sulphate, filtered and the solvent was removed *in vacuo*. The product was washed with hexane.

Yield 1.90 g, 73%
^{1}H NMR ($CDCl_3$): δ 7.28-7.14 (bm, 10H, Ar-H), 6.90 (m, 1H, NH), 5.11 (t, *J* = 8 Hz, 1H, CH), 4.60 (t, *J* = 8 Hz, 1H, CH_2), 4.05 (t, *J* = 8 Hz, 1H, CH_2).
^{13}C(^{1}H) NMR ($CDCl_3$): δ 158.4 (C=N), 143.1, 141.1 (Ar), 129.3, 129.1, 128.1, 126.9, 122.7, 119.8 (Ar), 75.1 (CH_2), 66.3 (CH).
MS (EI^+) m/z: 238 [M^+]
Anal. Calc'd for $C_{15}H_{14}N_2O$: C, 75.61; H, 5.92; N, 11.76. Found: C, 75.31; H, 5.95; N, 11.65.

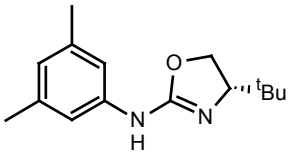
Synthesis of 2-phenylamino-4,4-dimethyloxazoline HL[3]



A mixture of two solutions, one of NaOH (1.32 g, 33.1 mmol) in water (2 mL), and a second of TsCl (3.8 g, 19.9 mmol) in THF (5 mL) was added dropwise *via* syringe over 5 minutes to a stirred solution of 1-(2-hydroxy-1,1-dimethylethyl)-3-phenylthiourea (2.97 g, 13.3 mmol) in THF (30 mL). After stirring overnight, water (20 mL) was added and the resultant suspension was extracted with Et_2O (3 x 20 mL). The combined organic layers were dried over magnesium sulphate, filtered and the solvent was removed *in vacuo*. The product was washed with hexane.

Yield: 2.09 g, 77%.
^{1}H NMR ($CDCl_3$): δ 7.26 (bm, 4H, Ar-H), 6.98 (bm, 1H, Ar-H), 6.30-4.20 (bm, 1H, NH), 4.02 (s, 2H, CH_2), 1.34 (s, 6H, CH_3).
^{13}C(^{1}H) NMR ($CDCl_3$): δ 155.8 (C=N), 128.9, 122.2, 120.6 (Ar), 78.7 (CH_2), 68.0 (CMe_2), 28.1 (CH_3).
MS (EI^+) m/z: 190 [M^+]
Anal. Calc'd for $C_{11}H_{14}N_2O$: C, 69.45; H, 7.42; N, 14.73. Found: C, 69.23; H, 7.45; N, 14.81.

Synthesis of (*S*) 2-(3,5-dimethyl)phenylamino-4-*tert*-butyloxazoline HL[4]



A mixture of two solutions, one of NaOH (0.54 g, 13.5 mmol) in water (2 mL), and a second of TsCl (1.12 g, 5.87 mmol) in THF (5 mL) was added dropwise *via* syringe over 5 minutes to a stirred solution of 1-hydroxy-2-[(3,5 dimethyl)phenylthiourea]-3,3-dimethylbutyl (1.50 g, 5.35 mmol) in THF (30 mL). After stirring overnight, water (20 mL) was added and the resultant suspension was extracted with Et_2O (3 x 20 mL). The combined organic layers were dried over magnesium sulphate, filtered and the solvent was removed *in vacuo*. The product was recrystallised from a minimum amount of hexane.

Yield = 1.01 g, 77 %.

^{1}H NMR ($CDCl_3$): δ 6.92 (s, 2H, Ar-H), 6.59 (s, 1H, Ar-H), 4.23 (t, *J* = 7 Hz, 1H, CH), 4.12, (t, *J* = 7 Hz, 1H, CH_2), 3.83-3.70 (m, 1H, CH_2), 2.28 (s, 6H, 2 x CH_3), 0.90 (s, 9H, ^{t}Bu).

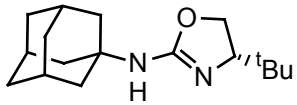
^{13}C NMR ($CDCl_3$): δ 154.5 (NHC(O)=N), 137.4 (Ar), 132.3, 123.0, 116.2, 69.9 (CH), 67.6 (CH_2), 32.9 (^{t}Bu), 24.4, 20.4 (CH_3).

IR (neat) ν cm^{-1}: 2956, 1681, 1599, 1475, 1402, 1365, 1247, 1078, 1008.

MS (CI^+) m/z: 247 (MH^+).

EA for $C_{15}H_{22}ON_2$, Calculated % C, 73.13; H, 9.00; N, 11.37. Found % C, 73.03; H, 8.94; N, 10.78.

Synthesis of (*S*) 2-(1-Adamantylamino)-4-*tert*-butyloxazoline HL^5



A mixture of two solutions, one of NaOH (0.63 g, 15.7 mmol) in water (2 mL), and a second of TsCl (1.31 g, 6.92 mmol) in THF (5 mL) was added dropwise *via* syringe over 5 minutes to a stirred solution of 1-hydroxy-2-(1-adamantylthiourea)-3,3-dimethylbutane (1.31 g, 6.92 mmol) in THF (30 mL). After stirring overnight, water (20 mL) was added and the resultant suspension was extracted with Et_2O (3 x 20 mL). The combined organic layers were dried over magnesium sulphate, filtered and the solvent was removed *in vacuo*. The product was washed with hot hexane (5 mL).

Yield = 1.52 g, 88%.

^{1}H NMR ($CDCl_3$): δ 3.91 - 4.05 (m, 1H, CH_2), 4.63 (dd, *J* = 7, 2 Hz, 1H, CH), 3.69 (dd, *J* = 8, 2 Hz, 1H, CH_2), 1.98 - 2.04 (m, 3H, 3 x Ad-CH), 1.83 - 1.91 (m, 6H, 3 x Ad-CH_2), 1.59 (s, 6H, 3 x Ad-CH_2), 0.78 (s, 9H, ^{t}Bu).

^{13}C NMR ($CDCl_3$): δ 156.1 (NHC(O)=N), 73.2 (CH), 66.6 (CH_2), 50.1 (Ad-C), 41.2 (Ad-CH_2), 35.4 (Ad-CH_2), 34.6 (^{t}Bu), 28.5 (Ad-CH), 24.6 (^{t}Bu).

MS (EI^+) m/z: 276 (M^+).

IR (neat) ν cm^{-1}: 3376, 2906, 1672, 1522, 1359, 1300, 1239, 1152, 1078, 1017, 979, 951, 672.

EA for $C_{17}H_{28}ON_2$, Calculated % C, 73.87; H, 10.21; N, 10.13. Found % C, 73.43; H, 10.08; N, 9.82.

Synthesis of [RuL^1(η-*p*-cymene)Cl]

THF (20 mL) was added to a Schlenk vessel containing [{RuCl(μ-Cl)(η^6-*p*-cymene)}$_2$] (335 mg, 0.69 mmol) and the sodium salt Na**L**^{1}.½THF (300 mg, 1.09 mmol). Stirring was continued overnight at ambient temperature followed by removal of solvent *in vacuo*. The resulting dark brown solid was extracted with toluene (2 x 20 mL) and the combined extracts were evaporated and dried *in vacuo* to give an orange solid. The product may be recrystallised from diethyl ether.

Yield = 410 mg, 77%.

^{1}H NMR (CD_2Cl_2): δ 7.36-7.30 (m, 2H, Ar-H), 7.26-7.24 (m, 2H, Ar-H), 7.01 (t, *J* = 7 Hz, 1H, Ar-H), 5.76 (d, *J* = 6 Hz, 1H, Ar-H), 5.61 (d, *J* = 6 Hz, 1H, Ar-H), 5.43 (m, 2H, Ar-H), 4.16 (dt, *J* = 9 Hz, 2H, CH_2), 3.32 (t, *J* = 10 Hz, 1H, CH), 2.89 (sept, *J* = 7 Hz, 1H, C*H*Me$_2$), 2.35 (s, 3H, CH_3), 1.36 (dd, *J* = 7 Hz, 6H, CH*Me*$_2$), 1.19 (s, 9H, ^{t}Bu).

^{13}C(^{1}H) NMR (CD_2Cl_2): δ 145.5, 128.8, 122.1, 121.2 (Ar), 99.5, 97.3, 80.8, 79.6, 78.9, 78.4 (*p*-cy), 70.1 (O-CH_2), 68.2 (N-CH), 33.3 (^{t}Bu), 32.0, (^{i}pr), 26.6 (^{t}Bu), 22.6 (^{i}pr), 22.5 (Ar-Me).

MS (EI$^+$) m/z: 488 [M$^+$]

Anal. Calc'd for $C_{23}H_{31}ClN_2ORu$: C, 56.60; H, 6.40; N, 5.74. Found: C, 56.62; H, 6.34; N, 5.26.

Synthesis of [Ru(η-C_6H_6)L^{1}Cl]

THF (20 mL) was added to a Schlenk vessel containing [{RuCl(μ-Cl)(C_6H_6)}$_2$] (300 mg, 0.69 mmol) at –78 °C. To the solution was added the sodium salt Na**L**^{1}.½THF (290 mg, 1.20 mmol) in THF (20 mL). Stirring was continued overnight at ambient temperature, followed by removal of solvent *in vacuo*. The resulting dark brown solid was extracted with toluene (2 x 20 mL) and the combined extracts were evaporated and dried *in vacuo* to give an orange solid. Single crystals were grown by cooling a hot solution in d^3-acetonitrile.

Yield = 347 mg, 67%.

^{1}H NMR (CD_2Cl_2): δ 7.25 (m, 4H, Ar-H), 6.94 (t, *J* = 7 Hz, 1H, Ar-H), 5.67 (s, 6H, Ar-H), 4.09 (dt, *J* = 9 Hz, 2H, CH_2), 3.26 (t, *J* = 9 Hz, 1H, CH), 1.18 (s, 9H, ^{t}Bu).

^{13}C(^{1}H) NMR (CD_2Cl_2): δ 145.0, 129.0, 121.9, 121.5 (Ar), 81.6 (C_6H_6), 70.3 (O-CH_2), 67.9 (N-CH), 33.2 (^{t}Bu), 32.0, 26.6 (^{t}Bu).

MS (EI$^+$) m/z: 432 [M$^+$]

Synthesis of [RuL^2(η-*p*-cymene)Cl]

THF (20 mL) was added to a Schlenk vessel containing [{RuCl(μ-Cl)(η^6-*p*-cymene)}$_2$] (370 mg, 0.73 mmol) and the sodium salt Na**L**^{2}.2THF (400 mg, 1.20 mmol). Stirring was continued overnight at ambient temperature followed by removal of solvent *in vacuo*. The resulting dark brown solid was extracted with toluene (2 x 20 mL) and the combined extracts were evaporated and dried *in vacuo* to give an orange solid. The product may be recrystallised from diethyl ether/pentane.

Yield = 489 mg, 80%.

^{1}H NMR (CD_2Cl_2): δ 7.59 (d, *J* = 7 Hz, 2H, Ar-H), 7.47 (t, *J* = 7 Hz, 2H, Ar-H), 7.40 (m, 1H, Ar-H), 7.25 (m, 4H, Ar-H), 6.95 (m, 1H, Ar-H), 5.53 (dd, 2H, Ar-H), 5.32 (m, 2H, Ar-H), 4.55 (dd, *J* = 8 Hz, 1H, CH_2), 4.46 (dd, *J* = 8 Hz, 1H, CH_2) 4.05 (dd, *J* = 8 Hz, 1H, CH), 2.73 (sept, *J* = 7 Hz, 1H, C*H*Me$_2$), 2.19 (s, 3H, CH_3), 1.21 (dd, *J* = 7 Hz, 6H, CH*Me*$_2$).

^{13}C(^{1}H) NMR (CD_2Cl_2): δ 144.8, 141.6, 129.0, 129.0, 128.1, 127.6, 122.1, 121.6 (Ar), 99.9, 96.8, 82.0, 78.9, 78.3 (*p*-cy), 75.7, (O-CH_2), 62.9 (N-CH), 32.0 (^{i}pr), 23.2 (^{i}pr), 22.0 (Ar-Me).

MS (EI$^+$) m/z: 508 [M$^+$]

Synthesis of [RuL^3(η-*p*-cymene)Cl]

THF (20 mL) was added to a Schlenk vessel containing [{RuCl(μ-Cl)(η^6-*p*-cymene)}$_2$] (400 mg, 1.31 mmol) and the sodium salt Na**L^3**.0.6THF (335 mg, 1.31 mmol). Stirring was continued overnight at ambient temperature followed by removal of solvent *in vacuo*. The resulting dark brown solid was extracted with toluene (2 x 20 mL) and the combined extracts were evaporated and dried *in vacuo* to give an orange solid. The product may be recrystallised from diethyl ether.

Yield = 95 mg, 17%

^{1}H NMR (CD_2Cl_2): δ 7.18 (m, 4H, Ar-H), 6.85 (m, 1H, Ar-H), 5.59 (dd, *J* = 6 Hz, 2H, Ar-H), 5.39 (dd, *J* = 6 Hz, 2H, Ar-H), 4.09 (d, *J* = 8 Hz, 1H, CH_2), 3.91 (d, *J* = 8 Hz, 1H, CH_2), 2.84 (sept, *J* = 7 Hz, 1H, C*H*Me$_2$), 2.26 (s, 3H, Ar-CH_3), 1.51 (s, 3H, C*Me*$_2$), 1.30 (dd, *J* = 5 Hz 6H, CH*Me*$_2$), 1.21 (s, 3H, C*Me*$_2$).

^{13}C(^{1}H) NMR (CD_2Cl_2): δ 145.4, 128.6, 121.2, 120.2 (Ar), 100.0, 96.6, 80.5 (*p*-cy), 80.4 (O-CH_2), 78.8, 78.1, 78.0 (*p*-cy), 61.9 (N*C*Me$_2$), 31.9 (^{i}pr), 29.9, 27.8, (^{i}pr), 22.7, 22.0 (NC*C*H$_3$), 19.2 (^{i}pr).

MS (EI$^+$) m/z: 460 [M$^+$]

Anal. Calc'd for $C_{21}H_{27}ClN_2ORu$: C, 54.83; H, 5.92; N, 6.09. Found: C, 52.27; H, 5.82; N, 5.32.

Synthesis of [ZrL$^1_2$(Bn)$_2$]

To a Schlenk vessel containing **HL^1** (0.20 g, 0.92 mmol) and Zr(Bn)$_4$ (0.21 g, 0.46 mmol) was added toluene (30 mL). The solution was stirred overnight in the dark, filtered and the solvent was removed *in vacuo*. The resulting pale yellow solid was washed with pentane (50 mL) leaving pure [ZrL$^1_2$(Bn)$_2$].

Yield = 0.28 g, 87 %.

^{1}H NMR (d^8-Toluene): δ 7.07 - 7.25 (m, 16H, Ar-H), 6.82 - 6.90 (m, 4H, Ar-H), 3.90 (dd, *J* = 8, 3 Hz, 2H, CH_2), 3.58 (t, *J* = 8 Hz, 2H, 2 x CH), 3.34 (dd, *J* = 8, 3 Hz, 2H, CH_2), 2.69 (d, *J* = 9 Hz, 2H, C*H*$_2$-Ar), 2.55 (d, *J* = 9 Hz, 2H, C*H*$_2$-Ar), 0.68 (s, 18H, 2 x ^{t}Bu).

^{13}C NMR (d^8-Toluene): δ 168.8 (NC(O)=N), 145.7 (Ar), 144.7, 129.1, 129.0, 128.3, 123.1, 123.0, 122.0, 76.8 (*C*H$_2$-Ar), 71.8 (CH_2), 70.9 (CH), 34.4 (^{t}Bu), 25.7.

MS (EI$^+$) m/z: 706 (M$^+$), 615 (M$^+$ - CH_2Ph), 524 (M$^+$ - 2 x CH_2Ph).

Synthesis of [ZrL$^1_2$(Np)$_2$]

To a Schlenk vessel containing **HL^1** (0.20 g, 0.92 mmol) and Zr(Np)$_4$ (0.17 g, 0.46 mmol) was added toluene (30mL). The solution was stirred overnight in the dark, filtered and the solvent removed *in vacuo* to leave a pale yellow solid. Recrystallisation from pentane of the complex by overnight cooling at -30^{o}C produced pale yellow crystals.

Yield = 0.28 g, 92%.

^{1}H NMR (d^6-Benzene): δ 7.51 (d, *J* = 7 Hz, 4H, Ar-H), 7.27 - 7.32 (m, 4H, Ar-H), 7.02 (t, *J* = 8 Hz, 2H, Ar-H), 4.08 - 4.12 (m, 2H, 2 x CH), 3.90 - 3.95 (m, 4H, 2 x CH_2), 1.98 (d, *J* = 9 Hz, 2H, C*H*$_2$-^{t}Bu), 1.86 (d, *J* = 9 Hz, 2H, C*H*$_2$-^{t}Bu), 1.43 (s, 18H, 2 x ^{t}Bu), 0.97 (s, 18H, 2 x ^{t}Bu).

^{13}C NMR (d^6-Benzene): δ 169.7 (NC(O)=N), 145.1 (Ar), 128.3, 123.1, 122.8, 91.1(*CH*$_2$-^{t}Bu), 71.5 (CH_2), 71.0 (CH), 36.3 (^{t}Bu-CH_2), 35.2, 35.0 (^{t}Bu), 25.7.

MS (EI$^+$) m/z: 595 (M$^+$ - $CH_2{}^t$Bu).

Synthesis of $[ZrL^4_2(Bn)_2]$

This was synthesised in an analogous way to $[ZrL^1_2(Bn)_2]$, using **HL^4** (0.25 g, 1.02 mmol) and $Zr(Bn)_4$ (2.31 g, 0.51 mmol).

Yield = 0.33g, 84%.

^{1}H NMR (d^8-Toluene): δ 7.21 - 7.08 (m, 8H, Ar-H), 6.99 - 7.04 (m, 2H, Ar-H), 6.95 - 6.99 (m, 2H, Ar-H), 6.83 - 6.89 (m, 2H, Ar-H), 6.87 (t, *J* = 8 Hz, 2H, Ar-H), 3.93 (dd, *J* = 7, 2 Hz, 2H, CH_2), 3.60 (t, *J* = 7 Hz, 2H, 2 x CH), 3.39 (dd, *J* = 7, 2 Hz, 2H, CH_2), 2.73 (d, *J*= 8 Hz, 2H, C*H*$_2$-Ar), 2.52 (d, *J* = 8 Hz, 2H, C*H*$_2$-Ar), 2.21 (s, 12H, 4 x CH_3-Ar), 0.71 (s, 18H, 2 x ^{t}Bu).

^{13}C NMR (d^8-Toluene): δ 169.2 (NC(O)=N), 146.9 (Ar), 144.3, 138.5, 129.0, 128.1, 125.7, 122.4, 121.6, 77.1(*C*H_2-Ar), 72.2(CH_2), 70.3(CH), 35.4 (^{t}Bu), 26.0, 21.8 (*C*H_3-Ar).

MS (EI^+) m/z: 671 (M^+ - CH_2Ph).

XRAY.

Synthesis of $[ZrL^4_2(Np)_2]$

This was synthesised in an analogous way to $[ZrL^1_2(Np)_2]$, using **HL^4** (0.20 g, 0.81 mmol) and $Zr(Np)_4$ (0.15 g, 0.41 mmol). No further purification was possible due to its high solubility in pentane and thermal sensitivity.

Yield = 0.26 g, 89 %.

^{1}H NMR (d^6-Benzene): δ 7.18 (s, 4H, Ar-H), 6.60 (s, 2H, Ar-H), 4.04 (dd, *J* = 6, 7 Hz, 2H, CH_2), 3.85 - 3.95 (m, 4H, 2 x CH, CH_2), 2.09 (s, 12H, 4 x CH_3), 1.91 (d, *J* = 6 Hz, 2H, C*H*$_2$-Ar), 1.78 (d, *J* = 7 Hz, 2H, C*H*$_2$-Ar), 1.36 (s, 18H, 2 x ^{t}Bu), 0.90 (s, 18H, 2 x ^{t}Bu).

^{13}C NMR (d^6-Benzene): δ 150.1 (NC(O)=N), 144.7 (Ar), 138.4, 125.1, 121.4, 92.1 (*C*H_2-^{t}Bu), 71.8 (CH_2), 71.3 (CH), 37.3 (^{t}Bu), 35.6, 35.3, 26.3, 22.0 (CH_3).

MS (CI^+) m/z: 652 (MH^+ - Np), 580 (MH^+ - 2 x Np).

Synthesis of $[ZrL^5_2(Bn)_2]$

This was synthesised in an analogous way to $[ZrL^1_2(Bn)_2]$, using **HL^6** (200 mg, 0.73 mmol) and $Zr(Bn)_4$ (165 mg, 0.36 mmol).

Yield = 0.26 g, 86%.

^{1}H NMR (d^8-Toluene): δ 7.22 (d, *J* = 8 Hz, 4H, Ar-H), 7.01 (t, *J* = 8 Hz, 4H, Ar-H), 6.64 (t, *J* = 8 Hz, 2H, Ar-H), 3.79 (dd, *J* = 7, 2 Hz, 2H, CH_2), 3.45 (t, *J* = 7 Hz, 2H, CH_2), 2.93 (dd, *J* = 7, 2 Hz, 2H, 2 x CH), 2.62 (d, *J*= 7 Hz, 2H, C*H*$_2$-Ar), 1.83 - 1.97 (m, 20H, C*H*$_2$-Ar, 6 x Ad-CH_2, 6 x Ad-CH), 1.40 - 1.54 (m, 12H, 6 x Ad-CH_2), 0.61 (s, 18H, 2 x ^{t}Bu).

^{13}C NMR (d^8-Toluene): δ 160.2 (NC(O)=N), 145.4 (Ar), 127.7, 126.2, 120.1, 72.9 (*C*H_2-Ar), 71.9 (CH_2), 69.2 (CH), 52.5 (C-Ad), 44.5 (CH_2-Ad), 36.9 (CH_2-Ad), 34.3 (^{t}Bu), 30.8 (CH-Ad), 25.8 (^{t}Bu).

MS(CI^+) m/z: 823 (MH^+).

MS (EI^+) m/z: 731 (M^+ - CH_2Ph).

Synthesis of $[ZrL^5_2(Np)_2]$

This was synthesised in an analogous way to $[ZrL^1_2(Np)_2]$, using **HL^6** (100 mg, 3.62 x 10^{-4} mol) and $Zr(Np)_4$ (68.0 mg, 1.81 x 10^{-4} mol). No further purification was possible due to its high solubility in pentane and thermal sensitivity.

Yield = 125 mg, 88%.

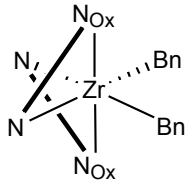
^{1}H NMR (d^{6}-Benzene): δ 4.07 - 4.19 (m, 4H, 2 x CH_2), 3.84 - 3.90 (m, 2H, 2 x CH), 1.92 - 2.20 (m, 18H, 6 x Ad-CH_2, 6 x Ad-CH), 1.53 - 1.73 (m, 14H, 6 x Ad-CH_2, C*H*$_2$-^{t}Bu), 1.35 (s, 18H, 2 x ^{t}Bu), 0.81 - 0.97 (m, 20H, C*H*$_2$^{t}Bu, 2 x ^{t}Bu).

^{13}C NMR (d^{6}-Benzene): δ 162.6 (NC(O)=N), 88.5 (*C*H_2-^{t}Bu), 70.2 (CH_2), 68.7 (CH), 52.2 (C-Ad), 42.9 (CH_2-Ad), 38.2 (^{t}Bu), 35.6 (CH_2-Ad), 34.8 (CH-Ad), 34.2 (^{t}Bu), 28.9 (^{t}Bu), 24.9 (^{t}Bu).

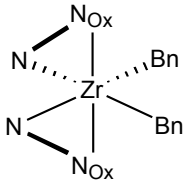
MS (CI^{+}) m/z: 783 (MH^{+}), 729 (MNH_4^{+} - CH_2^{t}Bu).

DFT Calculations

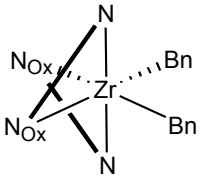
All DFT calculations employed the Amsterdam Density Functional (ADF) program version 2000.01. Geometries were optimised in the gas phase as follows: Zr: TZP[4p], N, CBz, DZP[1s], C, O: DZ[1s], H: DZ, default convergence except rad = 0.02, LDA geometry; PW91 energy.



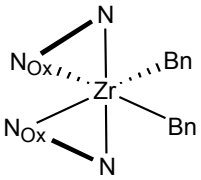
zr_dctc_calc.pdb
Δ–cis,trans,cis
See also IJM285.PDB
X-ray structure
rel energy = 0 kJ mol^{-1}



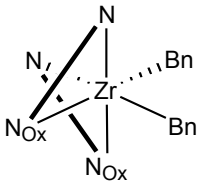
zr_lctc_calc.pdb
Λ–cis,trans,cis
+109 kJ mol^{-1}



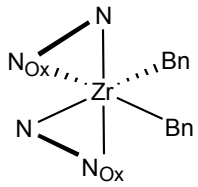
zr_dtcc_calc.pdb
Δ–trans,cis,cis
+84 kJ mol^{-1}



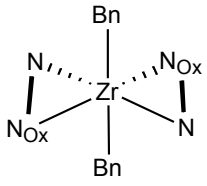
zr_ltcc_calc.pdb
Λ–trans,cis,cis
+107 kJ mol^{-1}



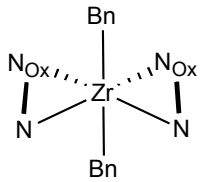
zr_dccc_calc.pdb
Δ–cis,cis,cis
+45.2 kJ mol^{-1}



zr_lccc_calc.pdb
Λ–cis,cis,cis
+111 kJ mol^{-1}



zr_ttt_calc.pdb
trans,trans,trans
+102 kJ mol^{-1}



zr_cct_calc.pdb
cis,cis,trans
+100 kJ mol^{-1}

Key to deposited structure files (.pdb) with configuration descriptors computed energies relative to the observed Δ-*cis,trans,cis*-[Zr$\mathbf{L}^4_2$(CH$_2$Ph)$_2$]
N_{Ox} = oxazolinyl N atom, N = amido N atom

Crystallographically determined structures (.pdb files)

.pdb file	Molecular formula	notes
arw1m.pdb	(S_{Ru},S_C)-[Ru(η-C_6H_6)$\mathbf{L}^1$Cl]	X-ray structure of Fig. 1
ijm285.pdb	Δ-*cis,trans,cis*-[Zr$\mathbf{L}^4_2$(CH$_2$Ph)$_2$]	X-ray structure of Fig. 2
ijm338m.pdb	[Ru(η-*p*-^{i}PrMeC$_6$H$_4$)$\mathbf{L}^3$Cl]	X-ray structure mentioned in footnote of manuscript.

Crystallographic Data Collection and Processing.

Data were collected on a Siemens SMART three-circle system with CCD area detector. Crystals were held at 180(2) K using an Oxford Cryosystem Cryostream Cooler. No crystal decay was detected. The structures were solved by direct methods using SHELXS (TREF) with additional light atoms found by Fourier methods. Hydrogen atoms were added at calculated positions and refined using a riding model with freely rotating methyl groups. Anisotropic displacement parameters were used for all non-H atoms; H-atoms were given isotropic displacement parameters equal to 1.2 (or 1.5 for methyl hydrogen atoms) times the equivalent isotropic displacement parameter of the atom to which the H-atom is attached. The absolute structure of the individual crystals of (S_{Ru},S_C)-[Ru(η-C_6H_6)**L**^{1}Cl] and [Zr**L**$^4{}_2$(CH_2Ph)$_2$] chosen were checked by refinement of a delta-f'' multiplier. Absolute structure parameters x = 0.03(4) and 0.02(7) respectively. Absolute configurations at C were shown to be correct by comparison with known absolute configuration of the compounds.

(S_{Ru}, S_C)-[Ru(η-C_6H_6)**L**^{1}Cl]

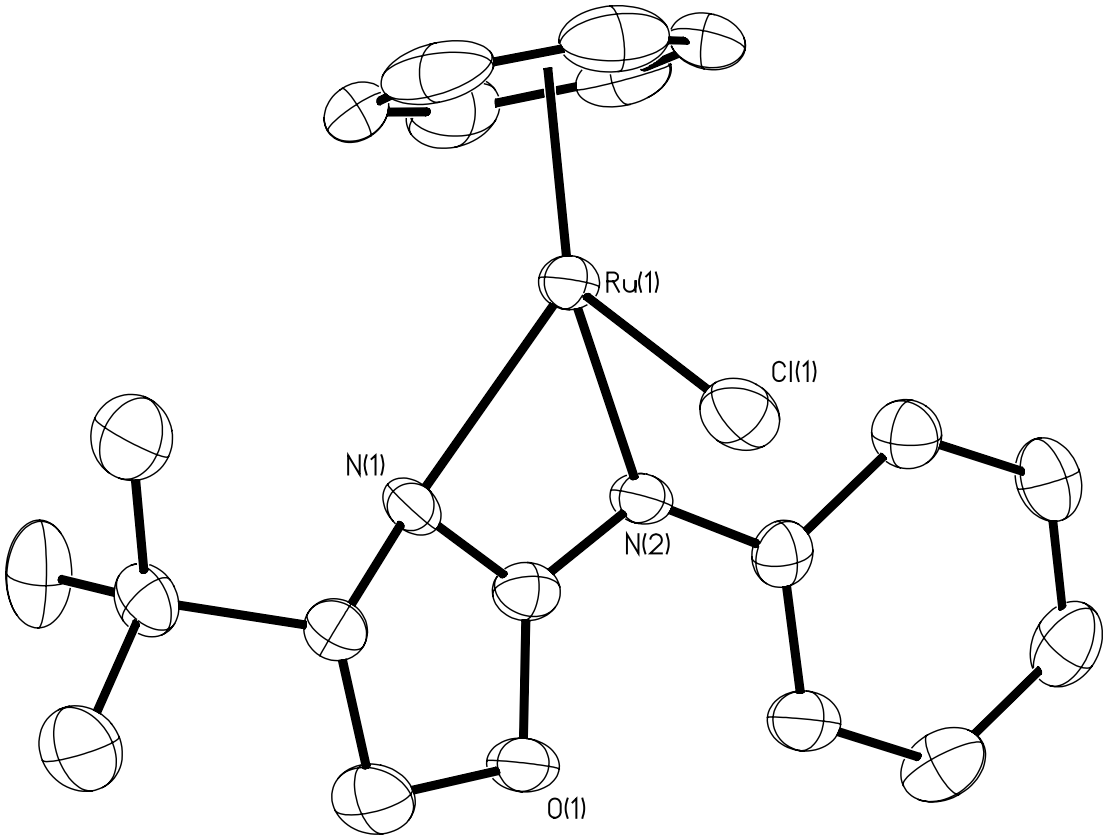


Table 1. Crystal data and structure refinement for arw1m (S_{Ru},S_C)-[Ru(η-C_6H_6)$\mathbf{L^1}$Cl].

Identification code	arw1m
Empirical formula	C19 H23 Cl N2 O Ru
Formula weight	431.91
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 10.1427(4) A alpha = 90 deg. b = 11.1134(4) A beta = 90 deg. c = 16.1543(6) A gamma = 90 deg.
Volume, Z	1820.91(12) A^3, 4
Density (calculated)	1.575 Mg/m^3
Absorption coefficient	1.015 mm^-1
F(000)	880
Crystal size	0.18 x 0.08 x 0.07 mm
Theta range for data collection	2.72 to 28.90 deg.
Limiting indices	-13<=h<=11, -15<=k<=14, -21<=l<=21
Reflections collected	11618
Independent reflections	4368 [R(int) = 0.0574]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.927992 and 0.711182
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4368 / 0 / 220
Goodness-of-fit on F^2	0.933
Final R indices [I>2sigma(I)]	R1 = 0.0368, wR2 = 0.0608
R indices (all data)	R1 = 0.0598, wR2 = 0.0662
Absolute structure parameter	0.03(4)
Largest diff. peak and hole	0.410 and -0.705 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for arw1m. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	5357(1)	2780(1)	8773(1)	24(1)
Cl(1)	5796(1)	1830(1)	7468(1)	38(1)
N(1)	4590(4)	1063(2)	9151(2)	24(1)
O(1)	2752(3)	311(2)	8510(2)	31(1)
C(4)	2325(4)	2875(4)	7997(2)	25(1)
C(5)	1137(4)	2276(4)	7819(2)	32(1)
C(6)	170(4)	2815(4)	7351(2)	37(1)
C(10)	5448(4)	-816(3)	9875(2)	30(1)
C(12)	5455(5)	-2178(4)	9780(3)	49(1)
C(3)	3503(4)	1281(3)	8726(3)	26(1)
C(7)	342(5)	3973(4)	7043(2)	39(1)
C(8)	1494(4)	4581(4)	7208(3)	36(1)
N(2)	3321(3)	2408(3)	8494(2)	24(1)
C(1)	4818(4)	-251(3)	9103(2)	24(1)
C(9)	2478(4)	4040(4)	7687(2)	31(1)
C(11)	6902(4)	-397(5)	9923(3)	51(1)
C(2)	3410(4)	-700(3)	8913(3)	37(1)
C(13)	4769(6)	-438(4)	10672(2)	51(1)
C(100)	5209(5)	4000(4)	9834(3)	47(1)
C(101)	5197(5)	4677(4)	9127(3)	41(1)
C(102)	6151(5)	4583(4)	8522(3)	39(1)
C(103)	7189(4)	3769(4)	8638(3)	48(1)
C(105)	6239(6)	3160(4)	9959(3)	55(2)
C(104)	7267(5)	3049(4)	9355(4)	58(2)

Table 3. Selected bond lengths [A] and angles [deg] for arw1m.

Ru(1)-N(1)	2.150(3)
Ru(1)-N(2)	2.154(3)
Ru(1)-C(105)	2.157(4)
Ru(1)-C(103)	2.170(4)
Ru(1)-C(104)	2.174(4)
Ru(1)-C(100)	2.190(4)
Ru(1)-C(101)	2.190(4)
Ru(1)-C(102)	2.197(4)
Ru(1)-Cl(1)	2.3997(11)
N(1)-Ru(1)-N(2)	62.71(12)
N(1)-Ru(1)-Cl(1)	85.74(8)
N(2)-Ru(1)-Cl(1)	84.83(8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [A] and angles [deg] for arw1m.

Ru(1)-N(1)	2.150(3)
Ru(1)-N(2)	2.154(3)
Ru(1)-C(105)	2.157(4)
Ru(1)-C(103)	2.170(4)
Ru(1)-C(104)	2.174(4)
Ru(1)-C(100)	2.190(4)
Ru(1)-C(101)	2.190(4)
Ru(1)-C(102)	2.197(4)
Ru(1)-Cl(1)	2.3997(11)
Ru(1)-C(3)	2.514(4)
N(1)-C(3)	1.320(5)
N(1)-C(1)	1.480(4)
O(1)-C(3)	1.365(4)
O(1)-C(2)	1.460(5)
C(4)-N(2)	1.391(5)
C(4)-C(9)	1.396(6)
C(4)-C(5)	1.407(5)
C(5)-C(6)	1.376(5)
C(5)-H(5A)	0.9500

C(6)-C(7)	1.391(6)
C(6)-H(6A)	0.9500
C(10)-C(13)	1.520(6)
C(10)-C(12)	1.522(5)
C(10)-C(1)	1.536(5)
C(10)-C(11)	1.548(6)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(3)-N(2)	1.320(4)
C(7)-C(8)	1.375(6)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.399(6)
C(8)-H(8A)	0.9500
C(1)-C(2)	1.544(6)
C(1)-H(1A)	1.0000
C(9)-H(9A)	0.9500
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(100)-C(101)	1.367(6)
C(100)-C(105)	1.416(7)
C(100)-H(10A)	1.0000
C(101)-C(102)	1.379(6)
C(101)-H(10B)	1.0000
C(102)-C(103)	1.401(6)
C(102)-H(10C)	1.0000
C(103)-C(104)	1.410(7)
C(103)-H(10D)	1.0000
C(105)-C(104)	1.433(8)
C(105)-H(10E)	1.0000
C(104)-H(10G)	1.0000

N(1)-Ru(1)-N(2)	62.71(12)
N(1)-Ru(1)-C(105)	94.10(15)
N(2)-Ru(1)-C(105)	128.38(18)
N(1)-Ru(1)-C(103)	142.01(18)
N(2)-Ru(1)-C(103)	153.85(17)
C(105)-Ru(1)-C(103)	68.6(2)
N(1)-Ru(1)-C(104)	108.76(17)
N(2)-Ru(1)-C(104)	166.19(19)
C(105)-Ru(1)-C(104)	38.6(2)
C(103)-Ru(1)-C(104)	37.89(19)
N(1)-Ru(1)-C(100)	107.61(14)
N(2)-Ru(1)-C(100)	102.50(16)
C(105)-Ru(1)-C(100)	38.02(18)
C(103)-Ru(1)-C(100)	79.87(18)
C(104)-Ru(1)-C(100)	68.8(2)
N(1)-Ru(1)-C(101)	138.89(16)
N(2)-Ru(1)-C(101)	99.69(15)
C(105)-Ru(1)-C(101)	67.08(18)
C(103)-Ru(1)-C(101)	66.59(18)
C(104)-Ru(1)-C(101)	79.69(18)
C(100)-Ru(1)-C(101)	36.37(15)
N(1)-Ru(1)-C(102)	174.11(14)
N(2)-Ru(1)-C(102)	119.23(15)
C(105)-Ru(1)-C(102)	80.40(16)
C(103)-Ru(1)-C(102)	37.42(17)
C(104)-Ru(1)-C(102)	68.16(18)
C(100)-Ru(1)-C(102)	66.72(16)
C(101)-Ru(1)-C(102)	36.64(16)
N(1)-Ru(1)-Cl(1)	85.74(8)
N(2)-Ru(1)-Cl(1)	84.83(8)
C(105)-Ru(1)-Cl(1)	142.17(18)
C(103)-Ru(1)-Cl(1)	88.61(13)
C(104)-Ru(1)-Cl(1)	105.98(17)
C(100)-Ru(1)-Cl(1)	166.56(13)
C(101)-Ru(1)-Cl(1)	131.83(13)
C(102)-Ru(1)-Cl(1)	99.89(12)
N(1)-Ru(1)-C(3)	31.68(12)
N(2)-Ru(1)-C(3)	31.68(11)
C(105)-Ru(1)-C(3)	117.80(17)
C(103)-Ru(1)-C(3)	166.76(15)
C(104)-Ru(1)-C(3)	140.39(17)
C(100)-Ru(1)-C(3)	112.46(16)

C(101)-Ru(1)-C(3)	126.16(16)
C(102)-Ru(1)-C(3)	150.84(15)
Cl(1)-Ru(1)-C(3)	79.68(10)
C(3)-N(1)-C(1)	106.6(3)
C(3)-N(1)-Ru(1)	89.5(2)
C(1)-N(1)-Ru(1)	143.5(3)
C(3)-O(1)-C(2)	103.8(3)
N(2)-C(4)-C(9)	118.2(4)
N(2)-C(4)-C(5)	124.3(4)
C(9)-C(4)-C(5)	117.4(4)
C(6)-C(5)-C(4)	121.1(4)
C(6)-C(5)-H(5A)	119.4
C(4)-C(5)-H(5A)	119.4
C(5)-C(6)-C(7)	120.7(4)
C(5)-C(6)-H(6A)	119.7
C(7)-C(6)-H(6A)	119.7
C(13)-C(10)-C(12)	111.2(3)
C(13)-C(10)-C(1)	112.8(3)
C(12)-C(10)-C(1)	109.0(3)
C(13)-C(10)-C(11)	107.8(4)
C(12)-C(10)-C(11)	107.5(4)
C(1)-C(10)-C(11)	108.3(3)
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N(2)-C(3)-N(1)	116.0(3)
N(2)-C(3)-O(1)	126.7(4)
N(1)-C(3)-O(1)	117.0(3)
N(2)-C(3)-Ru(1)	58.98(19)
N(1)-C(3)-Ru(1)	58.80(18)
O(1)-C(3)-Ru(1)	161.5(3)
C(8)-C(7)-C(6)	119.5(4)
C(8)-C(7)-H(7A)	120.3
C(6)-C(7)-H(7A)	120.3
C(7)-C(8)-C(9)	120.1(4)
C(7)-C(8)-H(8A)	119.9
C(9)-C(8)-H(8A)	119.9
C(3)-N(2)-C(4)	128.3(3)
C(3)-N(2)-Ru(1)	89.3(2)
C(4)-N(2)-Ru(1)	138.2(2)
N(1)-C(1)-C(10)	115.2(3)
N(1)-C(1)-C(2)	100.6(3)
C(10)-C(1)-C(2)	114.5(3)
N(1)-C(1)-H(1A)	108.7
C(10)-C(1)-H(1A)	108.7
C(2)-C(1)-H(1A)	108.7
C(4)-C(9)-C(8)	121.2(4)
C(4)-C(9)-H(9A)	119.4
C(8)-C(9)-H(9A)	119.4
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
O(1)-C(2)-C(1)	105.2(3)
O(1)-C(2)-H(2A)	110.7
C(1)-C(2)-H(2A)	110.7
O(1)-C(2)-H(2B)	110.7
C(1)-C(2)-H(2B)	110.7
H(2A)-C(2)-H(2B)	108.8
C(10)-C(13)-H(13A)	109.5
C(10)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(10)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(101)-C(100)-C(105)	119.3(5)
C(101)-C(100)-Ru(1)	71.8(2)
C(105)-C(100)-Ru(1)	69.7(2)
C(101)-C(100)-H(10A)	119.8
C(105)-C(100)-H(10A)	119.8
Ru(1)-C(100)-H(10A)	119.8
C(100)-C(101)-C(102)	122.9(5)
C(100)-C(101)-Ru(1)	71.8(2)
C(102)-C(101)-Ru(1)	71.9(2)
C(100)-C(101)-H(10B)	117.8

C(102)-C(101)-H(10B)	117.8
Ru(1)-C(101)-H(10B)	117.8
C(101)-C(102)-C(103)	118.8(4)
C(101)-C(102)-Ru(1)	71.4(2)
C(103)-C(102)-Ru(1)	70.2(2)
C(101)-C(102)-H(10C)	120.1
C(103)-C(102)-H(10C)	120.1
Ru(1)-C(102)-H(10C)	120.1
C(102)-C(103)-C(104)	121.2(4)
C(102)-C(103)-Ru(1)	72.3(2)
C(104)-C(103)-Ru(1)	71.2(3)
C(102)-C(103)-H(10D)	118.8
C(104)-C(103)-H(10D)	118.8
Ru(1)-C(103)-H(10D)	118.8
C(100)-C(105)-C(104)	119.7(4)
C(100)-C(105)-Ru(1)	72.3(2)
C(104)-C(105)-Ru(1)	71.3(3)
C(100)-C(105)-H(10E)	119.8
C(104)-C(105)-H(10E)	119.8
Ru(1)-C(105)-H(10E)	119.8
C(103)-C(104)-C(105)	118.0(4)
C(103)-C(104)-Ru(1)	70.9(3)
C(105)-C(104)-Ru(1)	70.0(3)
C(103)-C(104)-H(10G)	120.4
C(105)-C(104)-H(10G)	120.4
Ru(1)-C(104)-H(10G)	120.4

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for arw1m. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ru(1)	24(1)	20(1)	27(1)	1(1)	-4(1)	-2(1)
Cl(1)	49(1)	29(1)	36(1)	-5(1)	8(1)	-4(1)
N(1)	24(2)	21(2)	28(2)	8(1)	0(2)	-5(2)
O(1)	29(2)	22(1)	40(2)	1(1)	-8(1)	-6(1)
C(4)	30(2)	27(2)	20(2)	-3(2)	2(2)	2(2)
C(5)	32(2)	27(2)	36(2)	-1(2)	-3(2)	-5(2)
C(6)	29(2)	37(2)	44(2)	-10(2)	-7(2)	9(2)
C(10)	31(2)	25(2)	35(2)	7(2)	0(2)	5(2)
C(12)	54(3)	30(2)	62(3)	8(2)	-12(3)	8(3)
C(3)	25(2)	25(2)	26(2)	-4(2)	3(2)	-3(2)
C(7)	38(2)	41(2)	37(2)	-1(2)	-10(3)	13(3)
C(8)	41(3)	31(2)	36(3)	8(2)	2(2)	7(2)
N(2)	23(2)	18(2)	32(2)	3(1)	-6(1)	-3(1)
C(1)	25(2)	22(2)	27(2)	-1(1)	1(2)	2(2)
C(9)	30(2)	28(2)	34(2)	0(2)	0(2)	2(2)
C(11)	42(3)	50(3)	61(3)	14(3)	-15(3)	0(3)
C(2)	38(2)	21(2)	52(3)	-3(2)	-6(2)	6(2)
C(13)	65(3)	54(3)	35(2)	11(2)	-3(3)	17(3)
C(100)	49(3)	56(3)	37(3)	-16(2)	5(3)	-14(3)
C(101)	31(3)	36(2)	56(3)	-14(2)	-11(2)	-4(2)
C(102)	52(3)	25(2)	39(3)	-1(2)	-6(2)	-14(2)
C(103)	31(3)	52(3)	60(4)	-21(3)	12(2)	-13(2)
C(105)	87(4)	43(3)	36(3)	9(2)	-31(3)	-32(3)
C(104)	41(3)	30(3)	104(5)	-11(3)	-44(3)	6(2)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for arw1m.

	x	y	z	U(eq)
H(5A)	1000	1486	8026	38
H(6A)	-624	2392	7238	44
H(12A)	4548	-2481	9804	73
H(12B)	5972	-2538	10228	73
H(12C)	5848	-2393	9246	73
H(7A)	-331	4341	6721	46
H(8A)	1621	5369	6996	43
H(1A)	5393	-423	8614	29
H(9A)	3264	4472	7804	37
H(11A)	7336	-790	10393	77
H(11B)	6931	478	9998	77
H(11C)	7358	-614	9410	77
H(2A)	3435	-1408	8541	44
H(2B)	2947	-925	9430	44
H(13A)	3852	-717	10666	77
H(13B)	4786	441	10720	77
H(13C)	5230	-794	11146	77
H(10A)	4410	3975	10196	57
H(10B)	4364	5111	8984	49
H(10C)	6012	4966	7969	46
H(10D)	7779	3578	8159	57
H(10E)	6170	2556	10416	67
H(10G)	7916	2373	9388	70

[Zr$\mathbf{L}^4_2$(CH_2Ph)$_2$]

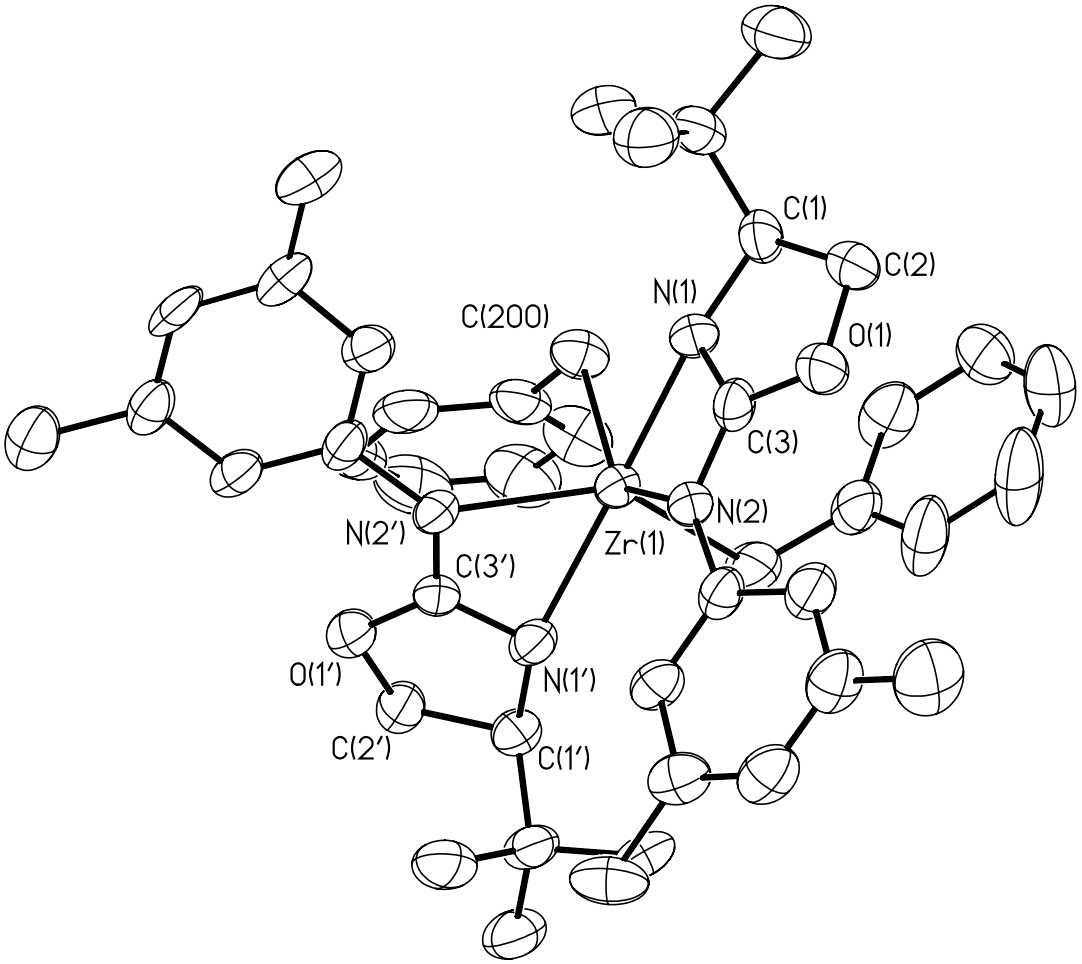


Table 1. Crystal data and structure refinement for ijm285. $[Zr\mathbf{L}^{4}_{2}(CH_2Ph)_2]$

Identification code	ijm285
Empirical formula	C44 H56 N4 O2 Zr
Formula weight	764.15
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system	Orthorhombic
Space group	P2(1)2(1)2(1)
Unit cell dimensions	a = 10.1903(2) A alpha = 90 deg. b = 17.3251(4) A beta = 90 deg. c = 25.7931(4) A gamma = 90 deg.
Volume, Z	4553.72(16) A^3, 4
Density (calculated)	1.115 Mg/m^3
Absorption coefficient	0.277 mm^-1
F(000)	1616
Crystal size	0.25 x 0.08 x 0.08 mm
Theta range for data collection	1.58 to 29.29 deg.
Limiting indices	-13<=h<=13, -23<=k<=15, -34<=l<=29
Reflections collected	29868
Independent reflections	11289 [R(int) = 0.1133]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.927997 and 0.742317
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11289 / 0 / 461
Goodness-of-fit on F^2	1.087
Final R indices [I>2sigma(I)]	R1 = 0.0892, wR2 = 0.1873
R indices (all data)	R1 = 0.1961, wR2 = 0.2390
Absolute structure parameter	0.02(7)
Extinction coefficient	0.0124(11)
Largest diff. peak and hole	0.712 and -0.474 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ijm285. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Zr(1)	2337(1)	2523(1)	11961(1)	36(1)
O(1)	917(5)	532(3)	12389(2)	52(1)
O(2)	5117(5)	3976(3)	11672(2)	42(1)
N(1)	1343(6)	1363(4)	11746(2)	41(2)
N(2)	2579(6)	1485(3)	12466(2)	38(1)
N(3)	3611(6)	3499(3)	12233(2)	38(2)
N(4)	4381(5)	2676(3)	11638(2)	38(2)
C(1)	220(7)	935(5)	11553(3)	42(2)
C(2)	-133(8)	436(6)	12017(3)	62(2)
C(3)	1648(7)	1118(4)	12209(3)	37(2)
C(4)	486(8)	476(5)	11050(3)	46(2)
C(5)	-765(9)	63(5)	10882(4)	68(3)
C(6)	1590(10)	-96(5)	11112(4)	65(3)
C(7)	886(9)	1023(5)	10615(3)	60(2)
C(8)	3055(7)	1332(4)	12973(3)	38(2)
C(9)	2556(8)	764(5)	13303(3)	49(2)
C(10)	3092(9)	653(5)	13794(3)	56(2)
C(11)	4137(9)	1115(5)	13953(3)	55(2)
C(12)	4624(8)	1704(5)	13625(3)	49(2)
C(13)	4078(7)	1785(4)	13136(3)	40(2)
C(14)	2580(11)	23(6)	14143(4)	83(3)
C(15)	5736(9)	2220(5)	13801(3)	64(3)
C(16)	3794(8)	4309(4)	12399(3)	41(2)
C(17)	4555(8)	4658(4)	11941(3)	46(2)
C(18)	4414(7)	3373(4)	11841(2)	34(2)
C(19)	4458(7)	4379(5)	12932(3)	43(2)
C(20)	3659(9)	3956(5)	13327(3)	52(2)
C(21)	4559(9)	5237(4)	13069(3)	56(2)
C(22)	5835(8)	4031(5)	12911(3)	56(2)
C(23)	5095(6)	2408(5)	11203(2)	38(2)
C(24)	6171(7)	2777(4)	10999(3)	40(2)
C(25)	6873(6)	2463(6)	10591(2)	43(2)
C(26)	6461(8)	1759(5)	10391(3)	47(2)
C(27)	5383(8)	1360(4)	10588(3)	42(2)
C(28)	4704(7)	1703(4)	10999(3)	41(2)
C(29)	8046(8)	2868(5)	10368(3)	55(2)
C(30)	4977(9)	608(5)	10374(3)	56(2)
C(31)	883(8)	3206(5)	12451(3)	59(2)
C(32)	-272(7)	2707(5)	12538(3)	49(2)
C(33)	-354(9)	2189(7)	12950(3)	77(3)
C(34)	-1420(10)	1708(7)	13007(4)	90(4)
C(35)	-2453(9)	1712(6)	12669(4)	72(3)
C(36)	-2411(8)	2201(5)	12261(3)	59(2)
C(37)	-1332(8)	2704(5)	12193(3)	57(3)
C(38)	1421(8)	2882(4)	11194(3)	45(2)
C(39)	1718(8)	3699(5)	11070(3)	48(2)
C(40)	844(10)	4294(6)	11202(4)	63(3)
C(41)	1088(11)	5062(6)	11063(4)	72(3)
C(42)	2207(12)	5235(5)	10816(4)	70(3)
C(43)	3095(10)	4680(6)	10687(3)	63(3)
C(44)	2862(9)	3911(5)	10808(3)	53(2)

Table 3. Selected bond lengths [A] and angles [deg] for ijm285.

Zr(1)-N(2)	2.233(5)
Zr(1)-N(3)	2.244(6)
Zr(1)-N(4)	2.259(5)
Zr(1)-C(38)	2.276(7)
Zr(1)-C(31)	2.278(7)
Zr(1)-N(1)	2.319(6)
Zr(1)-C(18)	2.596(7)
Zr(1)-C(3)	2.613(7)
O(1)-C(3)	1.341(9)
O(1)-C(2)	1.447(9)
O(2)-C(18)	1.340(8)
O(2)-C(17)	1.484(8)
N(1)-C(3)	1.305(8)
N(1)-C(1)	1.451(9)
N(2)-C(3)	1.321(9)
N(2)-C(8)	1.421(8)
N(3)-C(18)	1.319(8)
N(3)-C(16)	1.479(9)
N(4)-C(18)	1.316(9)
N(4)-C(23)	1.416(8)
N(2)-Zr(1)-N(3)	111.2(2)
N(2)-Zr(1)-N(4)	102.0(2)
N(3)-Zr(1)-N(4)	59.6(2)
N(2)-Zr(1)-C(38)	140.5(2)
N(3)-Zr(1)-C(38)	107.6(3)
N(4)-Zr(1)-C(38)	91.4(3)
N(2)-Zr(1)-C(31)	99.6(3)
N(3)-Zr(1)-C(31)	79.2(3)
N(4)-Zr(1)-C(31)	138.0(3)
C(38)-Zr(1)-C(31)	94.2(3)
N(2)-Zr(1)-N(1)	59.3(2)
N(3)-Zr(1)-N(1)	168.8(2)
N(4)-Zr(1)-N(1)	114.6(2)
N(2)-Zr(1)-C(18)	115.9(2)
N(3)-Zr(1)-C(18)	30.5(2)
N(4)-Zr(1)-C(18)	30.5(2)
C(38)-Zr(1)-C(18)	94.3(2)
C(31)-Zr(1)-C(18)	107.6(3)
N(1)-Zr(1)-C(18)	145.0(2)
N(1)-Zr(1)-C(3)	29.9(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [A] and angles [deg] for ijm285.

Zr(1)-N(2)	2.233(5)
Zr(1)-N(3)	2.244(6)
Zr(1)-N(4)	2.259(5)
Zr(1)-C(38)	2.276(7)
Zr(1)-C(31)	2.278(7)
Zr(1)-N(1)	2.319(6)
Zr(1)-C(18)	2.596(7)
Zr(1)-C(3)	2.613(7)
O(1)-C(3)	1.341(9)
O(1)-C(2)	1.447(9)
O(2)-C(18)	1.340(8)
O(2)-C(17)	1.484(8)
N(1)-C(3)	1.305(8)
N(1)-C(1)	1.451(9)
N(2)-C(3)	1.321(9)
N(2)-C(8)	1.421(8)
N(3)-C(18)	1.319(8)
N(3)-C(16)	1.479(9)
N(4)-C(18)	1.316(9)
N(4)-C(23)	1.416(8)
C(1)-C(2)	1.518(11)
C(1)-C(4)	1.545(10)
C(1)-H(1A)	1.0000
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(4)-C(6)	1.507(13)
C(4)-C(7)	1.525(11)
C(4)-C(5)	1.525(11)
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-C(13)	1.370(10)
C(8)-C(9)	1.397(10)
C(9)-C(10)	1.391(10)
C(9)-H(9A)	0.9500
C(10)-C(11)	1.394(12)
C(10)-C(14)	1.509(12)
C(11)-C(12)	1.415(12)
C(11)-H(11A)	0.9500
C(12)-C(13)	1.384(10)
C(12)-C(15)	1.514(11)
C(13)-H(13A)	0.9500
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(17)	1.537(10)
C(16)-C(19)	1.538(10)
C(16)-H(16A)	1.0000
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(19)-C(20)	1.496(11)
C(19)-C(22)	1.528(11)
C(19)-C(21)	1.531(10)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-C(24)	1.375(10)
C(23)-C(28)	1.387(11)
C(24)-C(25)	1.384(9)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.390(11)
C(25)-C(29)	1.500(11)

C(26)-C(27)	1.394(11)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.398(9)
C(27)-C(30)	1.475(11)
C(28)-H(28A)	0.9500
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(32)	1.478(11)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(33)	1.393(11)
C(32)-C(37)	1.400(10)
C(33)-C(34)	1.378(14)
C(33)-H(33A)	0.9500
C(34)-C(35)	1.366(13)
C(34)-H(34A)	0.9500
C(35)-C(36)	1.352(12)
C(35)-H(35A)	0.9500
C(36)-C(37)	1.414(12)
C(36)-H(36A)	0.9500
C(37)-H(37A)	0.9500
C(38)-C(39)	1.483(11)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-C(44)	1.397(11)
C(39)-C(40)	1.404(12)
C(40)-C(41)	1.401(13)
C(40)-H(40A)	0.9500
C(41)-C(42)	1.340(14)
C(41)-H(41A)	0.9500
C(42)-C(43)	1.362(14)
C(42)-H(42A)	0.9500
C(43)-C(44)	1.388(12)
C(43)-H(43A)	0.9500
C(44)-H(44A)	0.9500

N(2)-Zr(1)-N(3)	111.2(2)
N(2)-Zr(1)-N(4)	102.0(2)
N(3)-Zr(1)-N(4)	59.6(2)
N(2)-Zr(1)-C(38)	140.5(2)
N(3)-Zr(1)-C(38)	107.6(3)
N(4)-Zr(1)-C(38)	91.4(3)
N(2)-Zr(1)-C(31)	99.6(3)
N(3)-Zr(1)-C(31)	79.2(3)
N(4)-Zr(1)-C(31)	138.0(3)
C(38)-Zr(1)-C(31)	94.2(3)
N(2)-Zr(1)-N(1)	59.3(2)
N(3)-Zr(1)-N(1)	168.8(2)
N(4)-Zr(1)-N(1)	114.6(2)
C(38)-Zr(1)-N(1)	81.3(2)
C(31)-Zr(1)-N(1)	107.4(3)
N(2)-Zr(1)-C(18)	115.9(2)
N(3)-Zr(1)-C(18)	30.5(2)
N(4)-Zr(1)-C(18)	30.5(2)
C(38)-Zr(1)-C(18)	94.3(2)
C(31)-Zr(1)-C(18)	107.6(3)
N(1)-Zr(1)-C(18)	145.0(2)
N(2)-Zr(1)-C(3)	30.3(2)
N(3)-Zr(1)-C(3)	141.4(2)
N(4)-Zr(1)-C(3)	116.6(2)
C(38)-Zr(1)-C(3)	110.9(3)
C(31)-Zr(1)-C(3)	100.0(3)
N(1)-Zr(1)-C(3)	29.9(2)
C(18)-Zr(1)-C(3)	140.9(2)
C(3)-O(1)-C(2)	105.6(6)
C(18)-O(2)-C(17)	105.2(5)
C(3)-N(1)-C(1)	109.5(6)
C(3)-N(1)-Zr(1)	87.6(4)
C(1)-N(1)-Zr(1)	150.4(5)
C(3)-N(2)-C(8)	128.2(6)
C(3)-N(2)-Zr(1)	91.0(4)
C(8)-N(2)-Zr(1)	136.4(5)
C(18)-N(3)-C(16)	107.5(6)
C(18)-N(3)-Zr(1)	89.7(4)
C(16)-N(3)-Zr(1)	151.5(5)
C(18)-N(4)-C(23)	127.2(6)

C(18)-N(4)-Zr(1)	89.1(4)
C(23)-N(4)-Zr(1)	136.7(4)
N(1)-C(1)-C(2)	102.0(6)
N(1)-C(1)-C(4)	114.3(6)
C(2)-C(1)-C(4)	114.2(7)
N(1)-C(1)-H(1A)	108.7
C(2)-C(1)-H(1A)	108.7
C(4)-C(1)-H(1A)	108.7
O(1)-C(2)-C(1)	106.3(6)
O(1)-C(2)-H(2A)	110.5
C(1)-C(2)-H(2A)	110.5
O(1)-C(2)-H(2B)	110.5
C(1)-C(2)-H(2B)	110.5
H(2A)-C(2)-H(2B)	108.7
N(1)-C(3)-N(2)	118.2(7)
N(1)-C(3)-O(1)	115.5(7)
N(2)-C(3)-O(1)	126.1(6)
N(1)-C(3)-Zr(1)	62.4(4)
N(2)-C(3)-Zr(1)	58.7(4)
O(1)-C(3)-Zr(1)	159.8(5)
C(6)-C(4)-C(7)	106.6(8)
C(6)-C(4)-C(5)	110.2(7)
C(7)-C(4)-C(5)	107.8(7)
C(6)-C(4)-C(1)	112.4(7)
C(7)-C(4)-C(1)	110.2(6)
C(5)-C(4)-C(1)	109.5(7)
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(4)-C(6)-H(6A)	109.5
C(4)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(4)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(13)-C(8)-C(9)	119.6(7)
C(13)-C(8)-N(2)	115.8(6)
C(9)-C(8)-N(2)	124.6(7)
C(10)-C(9)-C(8)	120.6(8)
C(10)-C(9)-H(9A)	119.7
C(8)-C(9)-H(9A)	119.7
C(9)-C(10)-C(11)	119.3(8)
C(9)-C(10)-C(14)	120.4(9)
C(11)-C(10)-C(14)	120.3(8)
C(10)-C(11)-C(12)	120.3(7)
C(10)-C(11)-H(11A)	119.9
C(12)-C(11)-H(11A)	119.9
C(13)-C(12)-C(11)	118.5(8)
C(13)-C(12)-C(15)	120.9(8)
C(11)-C(12)-C(15)	120.6(7)
C(8)-C(13)-C(12)	121.8(7)
C(8)-C(13)-H(13A)	119.1
C(12)-C(13)-H(13A)	119.1
C(10)-C(14)-H(14A)	109.5
C(10)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(10)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(12)-C(15)-H(15A)	109.5
C(12)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(12)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
N(3)-C(16)-C(17)	102.4(5)
N(3)-C(16)-C(19)	112.9(6)
C(17)-C(16)-C(19)	115.7(6)
N(3)-C(16)-H(16A)	108.5
C(17)-C(16)-H(16A)	108.5
C(19)-C(16)-H(16A)	108.5

O(2)-C(17)-C(16)	103.9(5)
O(2)-C(17)-H(17A)	111.0
C(16)-C(17)-H(17A)	111.0
O(2)-C(17)-H(17B)	111.0
C(16)-C(17)-H(17B)	111.0
H(17A)-C(17)-H(17B)	109.0
N(4)-C(18)-N(3)	116.2(6)
N(4)-C(18)-O(2)	126.8(6)
N(3)-C(18)-O(2)	116.8(6)
N(4)-C(18)-Zr(1)	60.5(4)
N(3)-C(18)-Zr(1)	59.8(4)
O(2)-C(18)-Zr(1)	156.4(5)
C(20)-C(19)-C(22)	109.3(7)
C(20)-C(19)-C(21)	110.8(6)
C(22)-C(19)-C(21)	109.3(7)
C(20)-C(19)-C(16)	109.3(6)
C(22)-C(19)-C(16)	110.0(6)
C(21)-C(19)-C(16)	108.2(6)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(24)-C(23)-C(28)	119.6(6)
C(24)-C(23)-N(4)	124.1(7)
C(28)-C(23)-N(4)	116.2(6)
C(23)-C(24)-C(25)	121.4(7)
C(23)-C(24)-H(24A)	119.3
C(25)-C(24)-H(24A)	119.3
C(24)-C(25)-C(26)	118.0(7)
C(24)-C(25)-C(29)	121.3(8)
C(26)-C(25)-C(29)	120.7(7)
C(25)-C(26)-C(27)	122.6(6)
C(25)-C(26)-H(26A)	118.7
C(27)-C(26)-H(26A)	118.7
C(26)-C(27)-C(28)	117.0(7)
C(26)-C(27)-C(30)	121.5(7)
C(28)-C(27)-C(30)	121.5(8)
C(23)-C(28)-C(27)	121.3(7)
C(23)-C(28)-H(28A)	119.3
C(27)-C(28)-H(28A)	119.3
C(25)-C(29)-H(29A)	109.5
C(25)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(25)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(27)-C(30)-H(30A)	109.5
C(27)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(27)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-Zr(1)	107.4(5)
C(32)-C(31)-H(31A)	110.2
Zr(1)-C(31)-H(31A)	110.2
C(32)-C(31)-H(31B)	110.2
Zr(1)-C(31)-H(31B)	110.2
H(31A)-C(31)-H(31B)	108.5
C(33)-C(32)-C(37)	115.9(8)
C(33)-C(32)-C(31)	122.7(7)
C(37)-C(32)-C(31)	121.4(8)
C(34)-C(33)-C(32)	121.2(9)
C(34)-C(33)-H(33A)	119.4
C(32)-C(33)-H(33A)	119.4
C(35)-C(34)-C(33)	122.4(9)
C(35)-C(34)-H(34A)	118.8

C(33)-C(34)-H(34A)	118.8
C(36)-C(35)-C(34)	118.4(9)
C(36)-C(35)-H(35A)	120.8
C(34)-C(35)-H(35A)	120.8
C(35)-C(36)-C(37)	120.5(8)
C(35)-C(36)-H(36A)	119.8
C(37)-C(36)-H(36A)	119.8
C(32)-C(37)-C(36)	121.6(8)
C(32)-C(37)-H(37A)	119.2
C(36)-C(37)-H(37A)	119.2
C(39)-C(38)-Zr(1)	111.4(5)
C(39)-C(38)-H(38A)	109.4
Zr(1)-C(38)-H(38A)	109.4
C(39)-C(38)-H(38B)	109.4
Zr(1)-C(38)-H(38B)	109.4
H(38A)-C(38)-H(38B)	108.0
C(44)-C(39)-C(40)	117.0(8)
C(44)-C(39)-C(38)	121.7(8)
C(40)-C(39)-C(38)	121.3(8)
C(41)-C(40)-C(39)	121.5(10)
C(41)-C(40)-H(40A)	119.2
C(39)-C(40)-H(40A)	119.2
C(42)-C(41)-C(40)	119.0(10)
C(42)-C(41)-H(41A)	120.5
C(40)-C(41)-H(41A)	120.5
C(41)-C(42)-C(43)	121.6(9)
C(41)-C(42)-H(42A)	119.2
C(43)-C(42)-H(42A)	119.2
C(42)-C(43)-C(44)	120.6(9)
C(42)-C(43)-H(43A)	119.7
C(44)-C(43)-H(43A)	119.7
C(43)-C(44)-C(39)	120.2(9)
C(43)-C(44)-H(44A)	119.9
C(39)-C(44)-H(44A)	119.9

Symmetry transformations used to generate equivalent atoms:

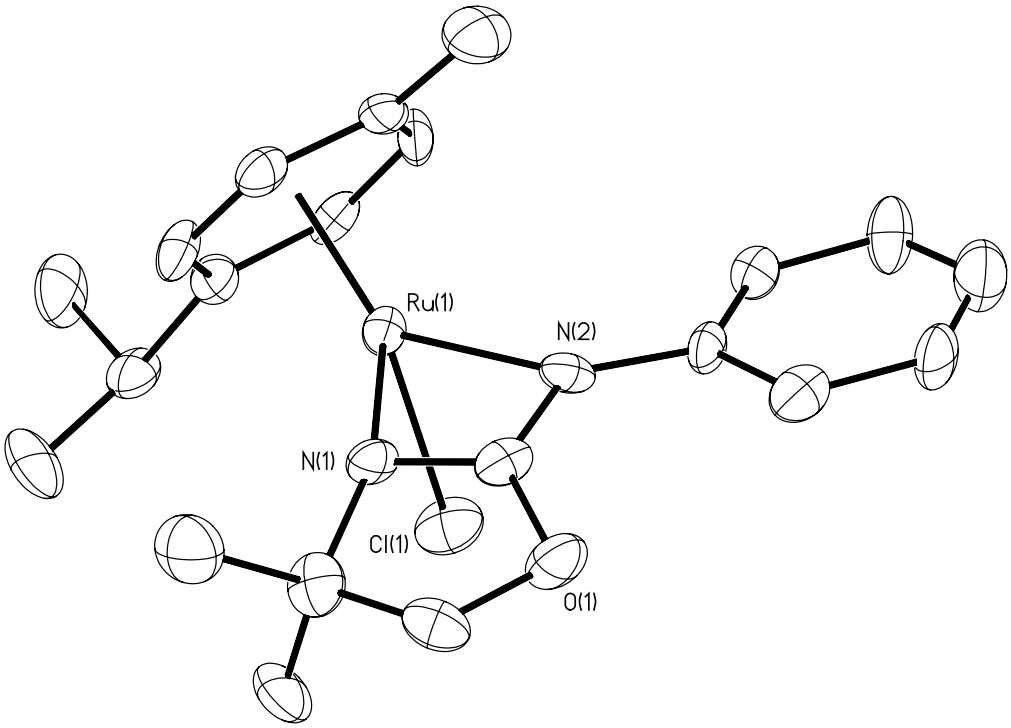
Table 5. Anisotropic displacement parameters (A^2 x 10^3) for ijm285.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

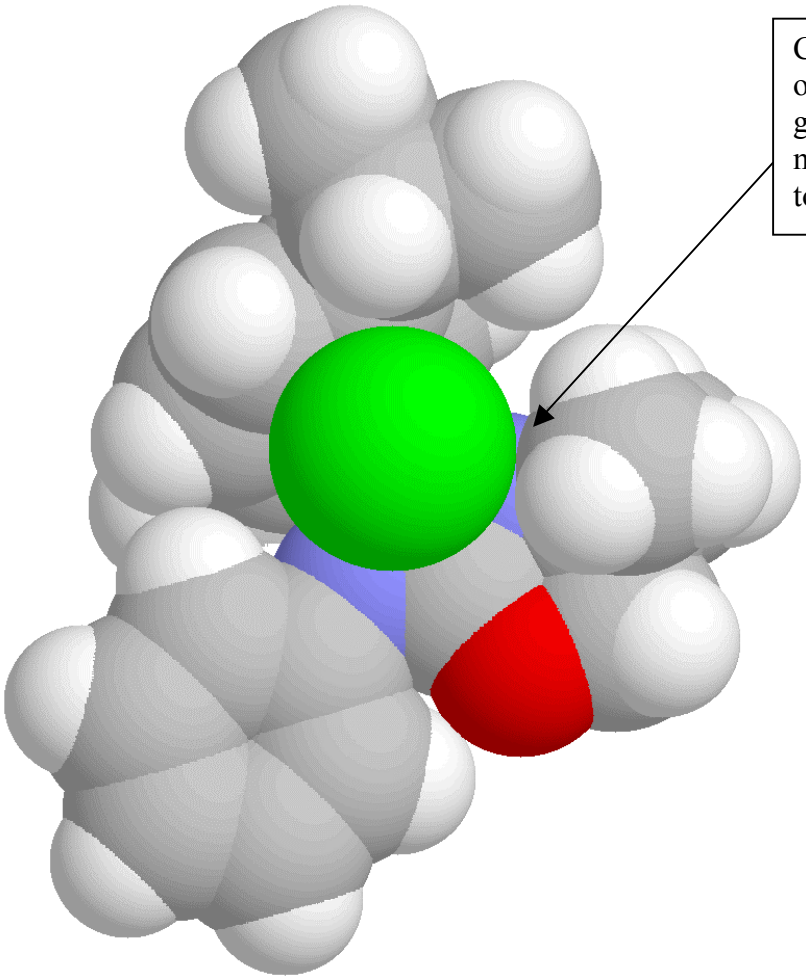
	U11	U22	U33	U23	U13	U12
Zr(1)	33(1)	46(1)	28(1)	-4(1)	0(1)	-2(1)
O(1)	51(4)	66(4)	38(3)	2(3)	-3(3)	-17(3)
O(2)	45(3)	41(3)	38(3)	-7(2)	6(2)	-4(2)
N(1)	40(4)	57(4)	27(3)	-1(3)	-4(3)	-9(3)
N(2)	33(3)	51(4)	29(3)	-2(3)	1(3)	-5(3)
N(3)	37(4)	46(4)	30(3)	-7(3)	2(3)	5(3)
N(4)	34(3)	51(5)	29(3)	-11(3)	3(2)	1(3)
C(1)	37(4)	55(5)	35(4)	5(4)	3(3)	-11(4)
C(2)	55(5)	88(7)	43(5)	-5(5)	-3(4)	-34(5)
C(3)	38(4)	41(5)	31(4)	6(3)	7(3)	-5(4)
C(4)	52(5)	47(5)	38(4)	7(4)	-10(4)	-15(4)
C(5)	73(7)	68(6)	62(6)	-8(5)	-10(5)	-18(5)
C(6)	76(8)	62(6)	56(6)	-7(5)	0(5)	-9(5)
C(7)	68(6)	75(7)	37(4)	-8(4)	-7(4)	-8(5)
C(8)	36(4)	49(5)	28(4)	6(3)	3(3)	4(3)
C(9)	43(5)	67(5)	38(4)	-3(4)	3(4)	7(4)
C(10)	54(6)	70(6)	44(5)	12(4)	-4(4)	11(5)
C(11)	57(6)	68(6)	41(5)	5(4)	-4(4)	18(5)
C(12)	53(5)	51(5)	44(5)	-9(4)	-5(4)	11(4)
C(13)	45(4)	46(5)	30(4)	4(3)	-4(3)	6(4)
C(14)	80(8)	113(8)	55(5)	28(5)	-9(6)	5(7)
C(15)	72(6)	60(6)	59(5)	-10(4)	-35(5)	4(4)
C(16)	40(4)	42(5)	42(4)	-12(4)	5(3)	-2(4)
C(17)	50(5)	46(5)	41(4)	-8(4)	10(4)	-10(4)
C(18)	31(4)	43(4)	27(4)	-3(3)	-4(3)	-3(3)
C(19)	46(5)	51(5)	31(4)	-9(3)	-4(3)	6(4)
C(20)	69(6)	58(5)	28(4)	-7(4)	1(4)	4(5)
C(21)	76(6)	49(5)	42(5)	-13(4)	2(5)	-8(4)
C(22)	53(5)	70(6)	45(5)	-8(4)	-12(4)	-4(4)
C(23)	33(3)	58(5)	25(3)	1(4)	3(2)	8(4)
C(24)	42(4)	48(5)	29(4)	-7(3)	3(3)	8(3)
C(25)	39(4)	62(5)	28(3)	2(5)	4(2)	9(5)
C(26)	55(5)	68(6)	18(3)	-8(4)	6(3)	14(4)
C(27)	55(5)	50(5)	21(3)	-2(3)	3(3)	18(4)
C(28)	41(4)	46(5)	35(4)	-6(3)	-1(3)	3(4)
C(29)	52(5)	69(6)	45(5)	7(4)	7(4)	8(4)
C(30)	79(7)	54(6)	36(4)	-8(4)	3(4)	10(5)
C(31)	40(5)	81(7)	55(5)	-36(5)	8(4)	0(5)
C(32)	31(4)	77(7)	39(4)	-10(4)	1(3)	10(4)
C(33)	41(5)	146(10)	44(5)	35(5)	7(4)	9(5)
C(34)	57(6)	133(10)	79(7)	60(7)	23(6)	10(6)
C(35)	46(6)	86(7)	85(7)	19(6)	17(5)	1(5)
C(36)	33(5)	85(6)	60(5)	-3(4)	-10(4)	-2(4)
C(37)	47(5)	81(8)	42(4)	11(4)	-1(4)	20(4)
C(38)	46(5)	43(5)	46(4)	2(4)	-10(4)	-1(4)
C(39)	47(5)	55(6)	43(5)	-1(4)	-16(4)	-9(4)
C(40)	62(7)	53(6)	74(6)	-5(5)	-12(5)	-3(5)
C(41)	74(8)	49(6)	93(8)	-17(5)	-11(6)	3(5)
C(42)	88(8)	42(5)	78(7)	1(5)	-21(6)	-14(6)
C(43)	71(7)	69(7)	49(5)	6(5)	-17(4)	-30(5)
C(44)	62(6)	66(6)	32(4)	-4(4)	-16(4)	-5(5)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for ijm285.

	x	y	z	U(eq)
H(1A)	-514	1305	11488	51
H(2A)	-979	603	12168	74
H(2B)	-208	-112	11912	74
H(5A)	-596	-227	10563	101
H(5B)	-1458	444	10819	101
H(5C)	-1046	-293	11156	101
H(6A)	1725	-371	10784	97
H(6B)	1367	-467	11385	97
H(6C)	2397	178	11206	97
H(7A)	1055	726	10299	90
H(7B)	1684	1302	10716	90
H(7C)	178	1393	10551	90
H(9A)	1845	451	13192	59
H(11A)	4525	1035	14284	66
H(13A)	4422	2164	12908	48
H(14A)	1848	-242	13972	124
H(14B)	2276	248	14470	124
H(14C)	3283	-349	14213	124
H(15A)	5943	2592	13526	95
H(15B)	6512	1905	13875	95
H(15C)	5473	2498	14115	95
H(16A)	2913	4563	12417	50
H(17A)	3962	4949	11708	55
H(17B)	5258	5007	12064	55
H(20A)	4079	4001	13667	77
H(20B)	3597	3411	13230	77
H(20C)	2777	4180	13342	77
H(21A)	4979	5294	13409	84
H(21B)	3678	5463	13081	84
H(21C)	5085	5503	12806	84
H(22A)	6252	4077	13252	84
H(22B)	6361	4307	12653	84
H(22C)	5776	3484	12815	84
H(24A)	6439	3258	11141	48
H(26A)	6932	1541	10109	56
H(28A)	3960	1450	11141	49
H(29A)	8192	3353	10555	83
H(29B)	7891	2979	10000	83
H(29C)	8821	2538	10403	83
H(30A)	5569	463	10090	85
H(30B)	4078	645	10241	85
H(30C)	5015	215	10646	85
H(31A)	1287	3351	12786	71
H(31B)	620	3684	12268	71
H(33A)	339	2167	13196	92
H(34A)	-1438	1360	13291	108
H(35A)	-3183	1379	12720	87
H(36A)	-3113	2208	12018	71
H(37A)	-1325	3047	11905	68
H(38A)	1762	2547	10914	54
H(38B)	458	2811	11212	54
H(40A)	68	4172	11389	76
H(41A)	470	5455	11144	87
H(42A)	2386	5757	10729	83
H(43A)	3881	4820	10513	75
H(44A)	3483	3528	10712	64

[Ru(η-*p*-^{i}PrMeC$_6$H$_4$)**L**^{3}Cl]





Close approach of oxazoline 4-methyl group to Cl atom as mentioned in footnote to manuscript.

Table 1. Crystal data and structure refinement for ijm338m. [Ru(η-*p*-^{i}PrMeC$_6$H$_4$)**L**^{3}Cl]

Identification code	ijm338m
Empirical formula	C21 H27 Cl N2 O Ru
Formula weight	459.97
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 10.2335(6)A alpha = 90 deg. b = 15.6579(9)A beta = 100.5710(10) deg. c = 12.9042(7)A gamma = 90 deg.
Volume, Z	2032.6(2) A^3, 4
Density (calculated)	1.503 Mg/m^3
Absorption coefficient	0.915 mm^-1
F(000)	944
Crystal size	0.3 x 0.15 x 0.1 mm
Theta range for data collection	2.07 to 25.00 deg.
Limiting indices	-12<=h<=11, -15<=k<=18, -14<=l<=15
Reflections collected	10126
Independent reflections	3544 [R(int) = 0.1540]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.927998 and 0.491667
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3544 / 0 / 240
Goodness-of-fit on F^2	1.131
Final R indices [I>2sigma(I)]	R1 = 0.0942, wR2 = 0.1697
R indices (all data)	R1 = 0.1432, wR2 = 0.1947
Largest diff. peak and hole	1.321 and -1.404 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ijm338m. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	8932(1)	1235(1)	7599(1)	23(1)
Cl(1)	7891(3)	2579(2)	7021(2)	37(1)
O(1)	9830(8)	1543(5)	4851(6)	36(2)
N(1)	8686(9)	899(6)	5992(7)	28(2)
N(2)	10427(8)	1649(6)	6726(7)	26(2)
C(1)	7832(12)	773(7)	4950(9)	36(3)
C(2)	8805(12)	1002(8)	4208(9)	38(3)
C(3)	9705(10)	1361(7)	5865(8)	26(2)
C(4)	6624(11)	1378(8)	4814(10)	41(3)
C(5)	7349(14)	-156(9)	4816(11)	53(4)
C(6)	11573(10)	2162(7)	6879(9)	26(2)
C(7)	11986(11)	2557(7)	7830(9)	29(3)
C(8)	13162(12)	3027(7)	8051(10)	38(3)
C(9)	13941(13)	3104(9)	7282(12)	52(4)
C(10)	13510(12)	2755(8)	6300(10)	38(3)
C(11)	12335(12)	2275(8)	6093(10)	36(3)
C(101)	11683(12)	232(9)	8748(10)	44(3)
C(102)	10256(10)	450(7)	8736(8)	28(3)
C(103)	9195(11)	-64(7)	8201(8)	31(3)
C(104)	7859(11)	169(7)	8147(9)	28(3)
C(105)	7505(10)	936(7)	8628(9)	28(3)
C(106)	8571(11)	1435(7)	9194(8)	28(3)
C(107)	9892(10)	1189(8)	9250(8)	29(2)
C(108)	6089(10)	1257(8)	8529(8)	30(2)
C(109)	5107(11)	816(9)	7657(10)	45(3)
C(110)	5635(12)	1143(9)	9568(10)	45(3)

Table 3. Selected bond lengths [A] and angles [deg] for ijm338m.

Ru(1)-N(1)	2.108(9)
Ru(1)-N(2)	2.159(9)
Ru(1)-C(103)	2.176(11)
Ru(1)-C(107)	2.177(10)
Ru(1)-C(106)	2.180(10)
Ru(1)-C(102)	2.185(11)
Ru(1)-C(104)	2.186(11)
Ru(1)-C(105)	2.197(11)
Ru(1)-Cl(1)	2.415(3)
Ru(1)-C(3)	2.514(10)
O(1)-C(3)	1.368(12)
O(1)-C(2)	1.479(14)
N(1)-C(3)	1.304(13)
N(1)-C(1)	1.476(14)
N(2)-C(3)	1.297(13)
N(2)-C(6)	1.405(13)
N(1)-Ru(1)-N(2)	62.0(3)
N(1)-Ru(1)-C(103)	95.9(4)
N(2)-Ru(1)-C(103)	114.5(4)
N(1)-Ru(1)-C(107)	154.8(4)
N(2)-Ru(1)-C(107)	106.5(3)
N(1)-Ru(1)-Cl(1)	87.0(3)
N(2)-Ru(1)-Cl(1)	83.8(2)
N(1)-Ru(1)-C(3)	31.2(3)
N(2)-Ru(1)-C(3)	31.1(3)
Cl(1)-Ru(1)-C(3)	81.4(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [A] and angles [deg] for ijm338m.

Ru(1)-N(1)	2.108(9)
Ru(1)-N(2)	2.159(9)
Ru(1)-C(103)	2.176(11)
Ru(1)-C(107)	2.177(10)
Ru(1)-C(106)	2.180(10)
Ru(1)-C(102)	2.185(11)
Ru(1)-C(104)	2.186(11)
Ru(1)-C(105)	2.197(11)
Ru(1)-Cl(1)	2.415(3)
Ru(1)-C(3)	2.514(10)
O(1)-C(3)	1.368(12)
O(1)-C(2)	1.479(14)
N(1)-C(3)	1.304(13)
N(1)-C(1)	1.476(14)
N(2)-C(3)	1.297(13)
N(2)-C(6)	1.405(13)
C(1)-C(5)	1.536(17)
C(1)-C(4)	1.542(16)
C(1)-C(2)	1.545(16)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-C(7)	1.370(15)
C(6)-C(11)	1.399(14)
C(7)-C(8)	1.395(15)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.387(17)
C(8)-H(8A)	0.9500
C(9)-C(10)	1.376(18)
C(9)-H(9A)	0.9500
C(10)-C(11)	1.403(16)
C(10)-H(10I)	0.9500
C(11)-H(11A)	0.9500
C(101)-C(102)	1.497(15)
C(101)-H(10J)	0.9800
C(101)-H(10K)	0.9800
C(101)-H(10L)	0.9800
C(102)-C(107)	1.417(16)
C(102)-C(103)	1.423(15)
C(103)-C(104)	1.404(15)
C(103)-H(10D)	1.0000
C(104)-C(105)	1.429(15)
C(104)-H(10H)	1.0000
C(105)-C(106)	1.429(15)
C(105)-C(108)	1.517(14)
C(106)-C(107)	1.395(15)
C(106)-H(10C)	1.0000
C(107)-H(10A)	1.0000
C(108)-C(110)	1.509(15)
C(108)-C(109)	1.529(16)
C(108)-H(10B)	1.0000
C(109)-H(10E)	0.9800
C(109)-H(10F)	0.9800
C(109)-H(10G)	0.9800
C(110)-H(11B)	0.9800
C(110)-H(11C)	0.9800
C(110)-H(11D)	0.9800

N(1)-Ru(1)-N(2)	62.0(3)
N(1)-Ru(1)-C(103)	95.9(4)
N(2)-Ru(1)-C(103)	114.5(4)
N(1)-Ru(1)-C(107)	154.8(4)
N(2)-Ru(1)-C(107)	106.5(3)
C(103)-Ru(1)-C(107)	67.4(4)
N(1)-Ru(1)-C(106)	162.5(4)
N(2)-Ru(1)-C(106)	135.1(4)
C(103)-Ru(1)-C(106)	80.1(4)
C(107)-Ru(1)-C(106)	37.3(4)
N(1)-Ru(1)-C(102)	117.9(4)
N(2)-Ru(1)-C(102)	96.2(4)
C(103)-Ru(1)-C(102)	38.1(4)
C(107)-Ru(1)-C(102)	37.9(4)

C(106)-Ru(1)-C(102)	68.8(4)
N(1)-Ru(1)-C(104)	98.7(4)
N(2)-Ru(1)-C(104)	147.6(4)
C(103)-Ru(1)-C(104)	37.6(4)
C(107)-Ru(1)-C(104)	79.7(4)
C(106)-Ru(1)-C(104)	67.8(4)
C(102)-Ru(1)-C(104)	68.8(4)
N(1)-Ru(1)-C(105)	124.6(4)
N(2)-Ru(1)-C(105)	173.0(4)
C(103)-Ru(1)-C(105)	68.7(4)
C(107)-Ru(1)-C(105)	68.4(4)
C(106)-Ru(1)-C(105)	38.1(4)
C(102)-Ru(1)-C(105)	82.7(4)
C(104)-Ru(1)-C(105)	38.0(4)
N(1)-Ru(1)-Cl(1)	87.0(3)
N(2)-Ru(1)-Cl(1)	83.8(2)
C(103)-Ru(1)-Cl(1)	160.7(3)
C(107)-Ru(1)-Cl(1)	115.2(3)
C(106)-Ru(1)-Cl(1)	91.4(3)
C(102)-Ru(1)-Cl(1)	151.9(3)
C(104)-Ru(1)-Cl(1)	123.1(3)
C(105)-Ru(1)-Cl(1)	93.9(3)
N(1)-Ru(1)-C(3)	31.2(3)
N(2)-Ru(1)-C(3)	31.1(3)
C(103)-Ru(1)-C(3)	110.7(4)
C(107)-Ru(1)-C(3)	135.6(3)
C(106)-Ru(1)-C(3)	164.7(4)
C(102)-Ru(1)-C(3)	112.6(4)
C(104)-Ru(1)-C(3)	127.4(4)
C(105)-Ru(1)-C(3)	155.1(4)
Cl(1)-Ru(1)-C(3)	81.4(3)
C(3)-O(1)-C(2)	103.7(8)
C(3)-N(1)-C(1)	108.2(9)
C(3)-N(1)-Ru(1)	91.8(7)
C(1)-N(1)-Ru(1)	150.8(7)
C(3)-N(2)-C(6)	130.4(9)
C(3)-N(2)-Ru(1)	89.7(6)
C(6)-N(2)-Ru(1)	138.7(7)
N(1)-C(1)-C(5)	110.7(10)
N(1)-C(1)-C(4)	110.5(9)
C(5)-C(1)-C(4)	109.5(10)
N(1)-C(1)-C(2)	101.1(9)
C(5)-C(1)-C(2)	112.4(10)
C(4)-C(1)-C(2)	112.4(10)
O(1)-C(2)-C(1)	104.9(8)
O(1)-C(2)-H(2A)	110.8
C(1)-C(2)-H(2A)	110.8
O(1)-C(2)-H(2B)	110.8
C(1)-C(2)-H(2B)	110.8
H(2A)-C(2)-H(2B)	108.8
N(2)-C(3)-N(1)	115.3(9)
N(2)-C(3)-O(1)	127.5(10)
N(1)-C(3)-O(1)	116.9(9)
N(2)-C(3)-Ru(1)	59.2(5)
N(1)-C(3)-Ru(1)	57.0(5)
O(1)-C(3)-Ru(1)	165.4(7)
C(1)-C(4)-H(4A)	109.5
C(1)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(1)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(1)-C(5)-H(5A)	109.5
C(1)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(1)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(7)-C(6)-C(11)	118.1(10)
C(7)-C(6)-N(2)	119.7(9)
C(11)-C(6)-N(2)	122.1(10)
C(6)-C(7)-C(8)	122.3(11)
C(6)-C(7)-H(7A)	118.9
C(8)-C(7)-H(7A)	118.9
C(9)-C(8)-C(7)	119.1(12)
C(9)-C(8)-H(8A)	120.4
C(7)-C(8)-H(8A)	120.4
C(10)-C(9)-C(8)	119.7(12)
C(10)-C(9)-H(9A)	120.1
C(8)-C(9)-H(9A)	120.1

C(9)-C(10)-C(11)	120.5(11)
C(9)-C(10)-H(10I)	119.8
C(11)-C(10)-H(10I)	119.8
C(6)-C(11)-C(10)	120.1(12)
C(6)-C(11)-H(11A)	120.0
C(10)-C(11)-H(11A)	120.0
C(102)-C(101)-H(10J)	109.5
C(102)-C(101)-H(10K)	109.5
H(10J)-C(101)-H(10K)	109.5
C(102)-C(101)-H(10L)	109.5
H(10J)-C(101)-H(10L)	109.5
H(10K)-C(101)-H(10L)	109.5
C(107)-C(102)-C(103)	116.5(10)
C(107)-C(102)-C(101)	121.4(10)
C(103)-C(102)-C(101)	122.2(11)
C(107)-C(102)-Ru(1)	70.8(6)
C(103)-C(102)-Ru(1)	70.6(6)
C(101)-C(102)-Ru(1)	128.2(8)
C(104)-C(103)-C(102)	121.8(11)
C(104)-C(103)-Ru(1)	71.6(6)
C(102)-C(103)-Ru(1)	71.3(6)
C(104)-C(103)-H(10D)	118.4
C(102)-C(103)-H(10D)	118.4
Ru(1)-C(103)-H(10D)	118.4
C(103)-C(104)-C(105)	121.2(10)
C(103)-C(104)-Ru(1)	70.8(6)
C(105)-C(104)-Ru(1)	71.4(6)
C(103)-C(104)-H(10H)	118.6
C(105)-C(104)-H(10H)	118.6
Ru(1)-C(104)-H(10H)	118.6
C(106)-C(105)-C(104)	116.8(10)
C(106)-C(105)-C(108)	119.3(10)
C(104)-C(105)-C(108)	123.8(10)
C(106)-C(105)-Ru(1)	70.3(6)
C(104)-C(105)-Ru(1)	70.6(6)
C(108)-C(105)-Ru(1)	127.5(8)
C(107)-C(106)-C(105)	121.1(10)
C(107)-C(106)-Ru(1)	71.2(6)
C(105)-C(106)-Ru(1)	71.6(6)
C(107)-C(106)-H(10C)	118.8
C(105)-C(106)-H(10C)	118.8
Ru(1)-C(106)-H(10C)	118.8
C(106)-C(107)-C(102)	122.5(9)
C(106)-C(107)-Ru(1)	71.4(6)
C(102)-C(107)-Ru(1)	71.3(6)
C(106)-C(107)-H(10A)	117.9
C(102)-C(107)-H(10A)	117.9
Ru(1)-C(107)-H(10A)	117.9
C(110)-C(108)-C(105)	109.3(9)
C(110)-C(108)-C(109)	109.4(10)
C(105)-C(108)-C(109)	113.6(10)
C(110)-C(108)-H(10B)	108.1
C(105)-C(108)-H(10B)	108.1
C(109)-C(108)-H(10B)	108.1
C(108)-C(109)-H(10E)	109.5
C(108)-C(109)-H(10F)	109.5
H(10E)-C(109)-H(10F)	109.5
C(108)-C(109)-H(10G)	109.5
H(10E)-C(109)-H(10G)	109.5
H(10F)-C(109)-H(10G)	109.5
C(108)-C(110)-H(11B)	109.5
C(108)-C(110)-H(11C)	109.5
H(11B)-C(110)-H(11C)	109.5
C(108)-C(110)-H(11D)	109.5
H(11B)-C(110)-H(11D)	109.5
H(11C)-C(110)-H(11D)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for ijm338m. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ru(1)	22(1)	21(1)	26(1)	1(1)	7(1)	-2(1)
Cl(1)	51(2)	22(1)	39(2)	0(1)	7(1)	9(1)
O(1)	45(5)	38(5)	24(4)	7(4)	6(4)	-2(4)
N(1)	26(5)	34(5)	24(5)	8(4)	7(4)	-1(4)
N(2)	22(5)	30(5)	25(5)	5(4)	4(4)	6(4)
C(1)	43(7)	23(6)	39(7)	-4(5)	1(6)	-2(5)
C(2)	37(7)	45(8)	29(6)	-4(6)	-1(5)	8(6)
C(3)	25(6)	31(6)	22(5)	2(5)	8(4)	7(5)
C(4)	22(6)	52(9)	48(7)	8(6)	3(5)	5(6)
C(5)	55(9)	44(8)	57(9)	2(7)	-1(7)	-9(7)
C(6)	19(6)	26(6)	34(6)	7(5)	12(5)	0(4)
C(7)	31(6)	25(6)	33(6)	5(5)	6(5)	-3(5)
C(8)	39(7)	26(6)	50(8)	-13(6)	8(6)	-15(5)
C(9)	33(7)	49(8)	74(10)	10(8)	12(7)	-8(6)
C(10)	32(7)	40(7)	45(8)	11(6)	17(6)	-6(6)
C(11)	37(7)	36(7)	40(7)	14(6)	18(6)	11(5)
C(101)	35(7)	53(8)	42(7)	7(6)	4(6)	13(6)
C(102)	24(6)	39(7)	24(6)	12(5)	8(5)	2(5)
C(103)	37(7)	34(6)	24(6)	8(5)	13(5)	1(5)
C(104)	28(6)	21(6)	36(6)	3(5)	7(5)	0(5)
C(105)	21(6)	28(6)	36(6)	4(5)	8(5)	3(4)
C(106)	38(7)	25(6)	22(5)	3(5)	9(5)	-5(5)
C(107)	15(5)	38(6)	31(6)	0(6)	2(4)	-19(5)
C(108)	24(6)	27(6)	41(6)	6(6)	8(5)	0(5)
C(109)	17(6)	54(9)	65(9)	3(7)	8(6)	7(5)
C(110)	27(6)	50(8)	63(8)	4(7)	17(6)	-2(6)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for ijm338m.

	x	y	z	U(eq)
H(2A)	9208	480	3969	45
H(2B)	8342	1317	3583	45
H(4A)	6930	1972	4828	61
H(4B)	6133	1285	5388	61
H(4C)	6040	1262	4137	61
H(5A)	8116	-538	4857	80
H(5B)	6765	-223	4128	80
H(5C)	6857	-301	5376	80
H(7A)	11451	2510	8356	35
H(8A)	13428	3289	8721	46
H(9A)	14767	3397	7433	62
H(10I)	14013	2841	5759	45
H(11A)	12055	2025	5417	43
H(10J)	12217	391	9431	65
H(10K)	12001	546	8186	65
H(10L)	11767	-383	8635	65
H(10D)	9406	-522	7718	37
H(10H)	7163	-130	7628	33
H(10C)	8379	2026	9417	34
H(10A)	10600	1620	9503	34
H(10B)	6083	1882	8367	37
H(10E)	5464	819	7002	68
H(10F)	4257	1121	7546	68
H(10G)	4971	225	7863	68
H(11B)	6264	1425	10127	68
H(11C)	5593	533	9726	68
H(11D)	4751	1397	9525	68