Supplementary material (ESI) for Dalton Transactions

List of Supplementary Information

Syntheses of Novel Di- and Trinucleating Ligands having Triethylbenzene Core with N,N-Bidentate Tethers. Their Complexation toward Pd and Rh Organometallic Fragments.

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Experimental procedures for X-ray crystallography ($\mathbf{L}^{\mathbf{pypz3}}$).

Data Collection

A white prism crystal of $C_{39}H_{39}N_9$ having approximate dimensions of 0.20 x 0.10 x 0.10 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS IV imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 oscillations that were exposed for 180 seconds. The crystal-to-detector distance was 110.00 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive monoclinic cell with dimensions:

a = 11.3126(6) Å

b = 26.386(2) Å β = 109.579(4)°

c = 12.2108(10) Å

V = 3434.1(5) Å^3

For Z = 4 and F.W. = 633.80, the calculated density is 1.226 g/cm^3. The systematic absences of:

h0l: h+l ± 2n

0k0: k ± 2n

uniquely determine the space group to be:

$P2_1/n$ (#14)

The data were collected at a temperature of -60 ± 1°C to a maximum 2θ value of 55.0°. A total of 60 oscillation images were collected. A sweep of data was done using ω oscillations from 0.0 to 180.0° in 3.0° steps. The exposure rate was 499.8 [sec./°]. The crystal-to-detector distance was 110.00 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 26954 reflections that were collected, 7758 were unique (R_{int} = 0.061).

The linear absorption coefficient, μ, for Mo-Kα radiation is 0.756 cm^{-1}. The data were corrected for Lorentz and polarization effects. A correction for secondary extinction[1] was applied (coefficient = 0.037500).

Structure Solution and Refinement

The structure was solved by direct methods[2] and expanded using Fourier techniques[3]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined isotropically. The

final cycle of full-matrix least-squares refinement[4] on F^2 was based on 7758 observed reflections and 591 variable parameters and converged (largest parameter shift was 0.03 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0457$$

$$wR2 = [\, \Sigma \, (\, w \, (Fo^2 - Fc^2)^2 \,) / \, \Sigma \, w(Fo^2)^2]^{1/2} = 0.1221$$

The standard deviation of an observation of unit weight[5] was 1.03. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.27 and -0.22 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[6]. Anomalous dispersion effects were included in Fcalc[7]; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley[8]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[9]. All calculations were performed using the CrystalStructure[10,11] crystallographic software package except for refinement, which was performed using SHELXL-97[12].

References

(1) Larson, A.C. (1970), Crystallographic Computing, 291-294. F.R. Ahmed, ed. Munksgaard, Copenhagen (equation 22, with V replaced by the cell volume).

(2) SIR92: Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M., Polidori, G., and Camalli, M. (1994) J. Appl. Cryst., 27, 435.

(3) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(4) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(5) Standard deviation of an observation of unit weight:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where N_o = number of observations

N_v = number of variables

(6) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(7) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(8) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).
(9) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).
(10) CrystalStructure 3.7.0: Crystal Structure Analysis Package, Rigaku and Rigaku/MSC (2000-2005). 9009 New Trails Dr. The Woodlands TX 77381 USA.
(11) CRYSTALS Issue 10: Watkin, D.J., Prout, C.K. Carruthers, J.R. & Betteridge, P.W. Chemical Crystallography Laboratory, Oxford, UK. (1996)
(12) SHELX97: Sheldrick, G.M. (1997).

Experimental procedures for X-ray crystallography (**1**).

Data Collection

An yellow prism crystal of $C_{51}H_{63}N_{12}B_3F_{12}Pd_3O_6$ having approximate dimensions of 0.10 x 0.10 x 0.10 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS IV imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 oscillations that were exposed for 360 seconds. The crystal-to-detector distance was 110.00 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive triclinic cell with dimensions:

a	= 13.074(8) Å	α	= 105.76(4)°
b	= 15.005(9) Å	β	= 97.23(4)°
c	= 17.337(9) Å	γ	= 110.73(2)°
V	= 2966.6(29) Å^3		

For Z = 2 and F.W. = 1519.76, the calculated density is 1.701 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of -60 ± 1°C to a maximum 2θ value of 54.8°. A total of 36 oscillation images were collected. A sweep of data was done using ω oscillations from 0.0 to 180.0° in 5.0° steps. The exposure rate was 799.8 [sec./°]. The crystal-to-detector distance was

110.00 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 15780 reflections that were collected, 10416 were unique (R_{int} = 0.076).

The linear absorption coefficient, μ, for Mo-Kα radiation is 9.966 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined isotropically. The final cycle of full-matrix least-squares refinement[3] on F^2 was based on 10416 observed reflections and 689 variable parameters and converged (largest parameter shift was 0.00 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0752$$

$$wR2 = [\, \Sigma \, (\, w \, (Fo^2 - Fc^2)^2 \,) / \, \Sigma \, w(Fo^2)^2]^{1/2} = 0.2264$$

The standard deviation of an observation of unit weight[4] was 0.904. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.663 and -0.762 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9,10] crystallographic software package except for refinement, which was performed using SHELXL-97[11].

References

(1) SHELX97: Sheldrick, G.M. (1997).

(2) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where N_o = number of observations

N_V = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) CrystalStructure 3.7.0: Crystal Structure Analysis Package, Rigaku and Rigaku/MSC (2000-2005). 9009 New Trails Dr. The Woodlands TX 77381 USA.

(10) CRYSTALS Issue 10: Watkin, D.J., Prout, C.K. Carruthers, J.R. & Betteridge, P.W. Chemical Crystallography Laboratory, Oxford, UK. (1996)

(11) SHELX97: Sheldrick, G.M. (1997).

Experimental procedures for X-ray crystallography (**2**).

Data Collection

An orange prismatic crystal of $C_{65.5}H_{82.5}N_{11.5}B_3F_{12}Rh_3O_5$ having approximate dimensions of 0.10 x 0.10 x 0.10 mm was mounted on a glass fiber. All measurements were made on a Rigaku RAXIS IV imaging plate area detector with graphite monochromated Mo-Kα radiation.

Indexing was performed from 3 oscillations that were exposed for 180 seconds. The crystal-to-detector distance was 110.00 mm.

Cell constants and an orientation matrix for data collection corresponded to a primitive triclinic cell with dimensions:

a	= 14.304(3) Å	α	= 104.890(11)°
b	= 14.663(5) Å	β	= 90.88(2)°
c	= 18.456(6) Å	γ	= 108.688(16)°
V	= 3523.5(19) Å^3		

For Z = 2 and F.W. = 1680.09, the calculated density is 1.584 g/cm^3. Based on a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

P-1 (#2)

The data were collected at a temperature of -60 ± 1°C to a maximum 2θ value of 55.0°. A total of 36 oscillation images were collected. A sweep of data was done using ω oscillations from 0.0 to 180.0° in 5.0° steps. The exposure rate was 880.2 [sec./°]. The crystal-to-detector distance was 110.00 mm. Readout was performed in the 0.100 mm pixel mode.

Data Reduction

Of the 25478 reflections that were collected, 14223 were unique (R_{int} = 0.088).

The linear absorption coefficient, μ, for Mo-Kα radiation is 7.83 cm^{-1}. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined isotropically. The final cycle of full-matrix least-squares refinement[3] on F^2 was based on 14223 observed reflections and 895 variable parameters and converged (largest parameter shift was 0.014 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma \, ||Fo| - |Fc|| \, / \, \Sigma \, |Fo| = 0.0892$$

$$wR2 = [\Sigma (w (Fo^2 - Fc^2)^2) / \Sigma \, w(Fo^2)^2]^{1/2} = 0.2726$$

The standard deviation of an observation of unit weight[4] was 1.06. Unit weights were used. The maximum and minimum peaks on the final difference Fourier map corresponded to 1.61 and -2.17 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf'' were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[8]. All calculations were performed using the CrystalStructure[9,10] crystallographic software package except for refinement, which was performed using SHELXL-97[11].

References

(1) SHELX97: Sheldrick, G.M. (1997).

(2) DIRDIF99: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., de Gelder, R., Israel, R. and Smits, J.M.M.(1999). The DIRDIF-99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least Squares function minimized: (SHELXL97)

$\Sigma w(F_o^2-F_c^2)^2$ where w = Least Squares weights.

(4) Standard deviation of an observation of unit weight:

$[\Sigma w(F_o^2-F_c^2)^2/(N_o-N_v)]^{1/2}$

where N_o = number of observations

N_v = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) CrystalStructure 3.7.0: Crystal Structure Analysis Package, Rigaku and Rigaku/MSC (2000-2005). 9009 New Trails Dr. The Woodlands TX 77381 USA.

(10) CRYSTALS Issue 10: Watkin, D.J., Prout, C.K. Carruthers, J.R. & Betteridge, P.W. Chemical Crystallography Laboratory, Oxford, UK. (1996)

(11) SHELX97: Sheldrick, G.M. (1997).

Table S1. Crystallographic Data for $\mathbf{L}^{pypz3}$, **1**, and **2**.

	$\mathbf{L}^{pypz3}$	$\mathbf{L}^{pypz3}$-Pd(allyl) (**1**)	$\mathbf{L}^{pypz3}$-Rh(cod) (**2**)
formula	$C_{39}H_{39}N_9$	$C_{51}H_{63}B_3F_{12}N_{12}O_6Pd_3$	$C_{65}H_{81}B_3F_{12}N_{11}O_4Rh_3$ +0.5(CH_3NO_2)
formula weight	633.80	1519.76	1680.09
crystal system	monoclinic	triclinic	triclinic
space group	*P21/n*(#14)	*P*-1(#2)	*P*-1(#2)
a/Å	11.3126(6)	13.074(8)	14.304(3)
b/Å	26.386(2)	15.005(9)	14.663(5)
c/Å	12.211(1)	17.337(9)	18.456(6)
α/deg	90	105.76(4)	104.890(11)
β/deg	109.579(4)	97.23(4)	90.88(2)
γ/deg	90	110.73(2)	108.688(16)
V/Å^3	3434.1(5)	2967(3)	3523.5(19)
Z	4	2	2
d_{calc}/g·cm^{-3}	1.226	1.701	1.584
temp	-60	-60	-60
radiation	MoKα (λ = 0.71069 Å)	MoKα (λ = 0.71069 Å)	MoKα (λ = 0.71069 Å)
μ/cm^{-1}	7.60	9.96	7.83
diffractometer	Rigaku RAXIS IV	Rigaku RAXIS IV	Rigaku RAXIS IV
max 2θ/deg	55.0	55.0	55.0
reflections collected	27257	15780	25478
independent reflections	7173 [R(int) = 0.061]	10416 [R(int) = 0.0757]	14223 [R(int) = 0.0880]
no. of parameters refined	591	694	895
R1 (I > 2σ) %	4.57	7.52	8.92
wR_2 (All) %	12.2	22.64	27.26
goodness of fit	1.031	0.904	1.060

Table S2. Bond lengths [Å] for $\mathbf{L}^{\mathbf{pypz3}}$.

N(1)-N(2)	1.3482(13)
N(1)-C(16)	1.3497(16)
N(1)-C(13)	1.4711(15)
N(2)-C(18)	1.3357(16)
N(3)-C(19)	1.3365(17)
N(3)-C(23)	1.3399(18)
N(4)-N(5)	1.3488(14)
N(4)-C(24)	1.3502(18)
N(4)-C(14)	1.4641(16)
N(5)-C(26)	1.3417(16)
N(6)-C(27)	1.3431(17)
N(6)-C(31)	1.3436(17)
N(7)-N(8)	1.3504(18)
N(7)-C(32)	1.3523(18)
N(7)-C(15)	1.459(2)
N(8)-C(34)	1.3419(19)
N(9)-C(39)	1.311(3)
N(9)-C(35)	1.340(2)
C(1)-C(2)	1.4039(17)
C(1)-C(6)	1.4058(17)
C(1)-C(7)	1.5132(19)
C(2)-C(3)	1.4016(17)
C(2)-C(13)	1.5143(16)
C(3)-C(4)	1.4086(16)
C(3)-C(9)	1.5174(17)
C(4)-C(5)	1.4037(17)
C(4)-C(14)	1.5158(18)
C(5)-C(6)	1.3970(18)
C(5)-C(11)	1.5201(17)
C(6)-C(15)	1.5140(18)
C(7)-C(8)	1.527(2)
C(9)-C(10)	1.523(2)
C(11)-C(12)	1.533(2)
C(16)-C(17)	1.3689(18)
C(17)-C(18)	1.4040(18)
C(18)-C(19)	1.4741(16)
C(19)-C(20)	1.389(2)
C(20)-C(21)	1.3799(19)
C(21)-C(22)	1.371(2)
C(22)-C(23)	1.379(2)
C(24)-C(25)	1.364(2)
C(25)-C(26)	1.400(2)
C(26)-C(27)	1.4685(18)
C(27)-C(28)	1.393(2)
C(28)-C(29)	1.380(2)
C(29)-C(30)	1.383(2)
C(30)-C(31)	1.377(2)
C(32)-C(33)	1.351(3)
C(33)-C(34)	1.402(2)
C(34)-C(35)	1.462(3)
C(35)-C(36)	1.394(3)
C(36)-C(37)	1.372(3)
C(37)-C(38)	1.411(4)
C(38)-C(39)	1.364(4)

Table S3. Bond angles [deg] for $\mathbf{L}^{\mathbf{pypz3}}$.

N(2)-N(1)-C(16)	111.91(10)
N(2)-N(1)-C(13)	119.42(10)
C(16)-N(1)-C(13)	128.67(10)
C(18)-N(2)-N(1)	104.82(10)
C(19)-N(3)-C(23)	117.35(13)
N(5)-N(4)-C(24)	112.03(11)
N(5)-N(4)-C(14)	120.16(10)
C(24)-N(4)-C(14)	127.82(11)
C(26)-N(5)-N(4)	104.70(10)
C(27)-N(6)-C(31)	117.31(13)
N(8)-N(7)-C(32)	112.63(15)
N(8)-N(7)-C(15)	121.28(11)
C(32)-N(7)-C(15)	126.03(14)
C(34)-N(8)-N(7)	104.26(13)
C(39)-N(9)-C(35)	117.7(2)
C(2)-C(1)-C(6)	119.16(11)
C(2)-C(1)-C(7)	120.75(11)
C(6)-C(1)-C(7)	120.06(11)
C(3)-C(2)-C(1)	120.79(10)
C(3)-C(2)-C(13)	120.08(11)
C(1)-C(2)-C(13)	119.06(11)
C(2)-C(3)-C(4)	119.08(11)
C(2)-C(3)-C(9)	120.98(11)
C(4)-C(3)-C(9)	119.84(11)
C(5)-C(4)-C(3)	120.74(11)
C(5)-C(4)-C(14)	119.56(11)
C(3)-C(4)-C(14)	119.68(11)
C(6)-C(5)-C(4)	119.26(11)
C(6)-C(5)-C(11)	119.47(12)
C(4)-C(5)-C(11)	121.27(12)
C(5)-C(6)-C(1)	120.91(11)
C(5)-C(6)-C(15)	119.70(11)
C(1)-C(6)-C(15)	119.37(12)
C(1)-C(7)-C(8)	111.36(14)
C(3)-C(9)-C(10)	112.11(12)
C(5)-C(11)-C(12)	113.06(13)
N(1)-C(13)-C(2)	110.93(10)
N(4)-C(14)-C(4)	110.45(11)
N(7)-C(15)-C(6)	112.32(11)
N(1)-C(16)-C(17)	107.37(11)
C(16)-C(17)-C(18)	104.60(12)
N(2)-C(18)-C(17)	111.30(10)
N(2)-C(18)-C(19)	120.66(11)
C(17)-C(18)-C(19)	128.04(12)
N(3)-C(19)-C(20)	122.25(12)
N(3)-C(19)-C(18)	116.35(12)
C(20)-C(19)-C(18)	121.39(12)
C(21)-C(20)-C(19)	119.02(15)
C(22)-C(21)-C(20)	119.40(15)
C(21)-C(22)-C(23)	117.89(13)
N(3)-C(23)-C(22)	124.09(15)
N(4)-C(24)-C(25)	107.12(13)
C(24)-C(25)-C(26)	105.22(13)
N(5)-C(26)-C(25)	110.93(12)
N(5)-C(26)-C(27)	120.77(12)
C(25)-C(26)-C(27)	128.30(13)
N(6)-C(27)-C(28)	122.81(12)
N(6)-C(27)-C(26)	115.50(12)
C(28)-C(27)-C(26)	121.69(12)
C(29)-C(28)-C(27)	118.63(14)
C(28)-C(29)-C(30)	119.12(15)
C(31)-C(30)-C(29)	118.61(14)
N(6)-C(31)-C(30)	123.52(14)
C(33)-C(32)-N(7)	106.42(16)
C(32)-C(33)-C(34)	106.20(15)
N(8)-C(34)-C(33)	110.49(17)
N(8)-C(34)-C(35)	121.16(15)
C(33)-C(34)-C(35)	128.34(16)
N(9)-C(35)-C(36)	122.03(19)
N(9)-C(35)-C(34)	115.46(17)
C(36)-C(35)-C(34)	122.50(16)
C(37)-C(36)-C(35)	119.8(2)
C(36)-C(37)-C(38)	117.4(3)
C(39)-C(38)-C(37)	118.3(3)
N(9)-C(39)-C(38)	124.8(3)

Symmetry transformations used to generate equivalent atoms:

Table S4. Bond lengths [Å] for **1**.

Pd(1)-N(2)	2.105(7)
Pd(1)-N(3)	2.117(9)
Pd(1)-C(40)	2.134(11)
Pd(1)-C(41)	2.134(19)
Pd(1)-C(42)	2.149(11)
Pd(1)-C(41A)	2.20(3)
Pd(2)-N(5)	2.078(7)
Pd(2)-C(43)	2.119(13)
Pd(2)-N(6)	2.120(7)
Pd(2)-C(44A)	2.13(3)
Pd(2)-C(45)	2.135(9)
Pd(2)-C(44)	2.19(2)
Pd(3)-C(47)	2.10(3)
Pd(3)-C(48)	2.107(11)
Pd(3)-C(47A)	2.12(2)
Pd(3)-N(8)	2.128(7)
Pd(3)-N(9)	2.140(9)
Pd(3)-C(46)	2.152(13)
N(1)-C(16)	1.345(11)
N(1)-N(2)	1.396(9)
N(1)-C(13)	1.474(11)
N(2)-C(18)	1.361(11)
N(3)-C(23)	1.361(12)
N(3)-C(19)	1.369(12)
N(4)-C(24)	1.353(12)
N(4)-N(5)	1.361(10)
N(4)-C(14)	1.467(10)
N(5)-C(26)	1.378(10)
N(6)-C(31)	1.327(12)
N(6)-C(27)	1.392(12)
N(7)-N(8)	1.329(9)
N(7)-C(32)	1.346(11)
N(7)-C(15)	1.481(10)
N(8)-C(34)	1.340(12)
N(9)-C(35)	1.324(13)
N(9)-C(39)	1.326(13)
C(1)-C(2)	1.403(11)
C(1)-C(6)	1.426(12)
C(1)-C(7)	1.503(12)
C(2)-C(3)	1.430(13)
C(2)-C(13)	1.496(12)
C(3)-C(4)	1.410(12)
C(3)-C(9)	1.521(11)
C(4)-C(5)	1.390(12)
C(4)-C(14)	1.523(12)
C(5)-C(6)	1.405(13)
C(5)-C(11)	1.509(13)
C(6)-C(15)	1.520(11)
C(7)-C(8)	1.523(12)
C(9)-C(10)	1.549(14)
C(11)-C(12)	1.527(13)
C(16)-C(17)	1.365(12)
C(17)-C(18)	1.391(12)
C(18)-C(19)	1.467(12)
C(19)-C(20)	1.350(13)
C(20)-C(21)	1.374(14)
C(21)-C(22)	1.362(15)
C(22)-C(23)	1.365(16)
C(24)-C(25)	1.367(13)
C(25)-C(26)	1.391(13)
C(26)-C(27)	1.414(13)
C(27)-C(28)	1.404(12)
C(28)-C(29)	1.404(15)
C(29)-C(30)	1.351(16)
C(30)-C(31)	1.436(15)
C(32)-C(33)	1.359(13)
C(33)-C(34)	1.403(13)
C(34)-C(35)	1.500(13)
C(35)-C(36)	1.377(15)
C(36)-C(37)	1.363(16)
C(37)-C(38)	1.38(2)
C(38)-C(39)	1.378(19)
C(40)-C(41A)	1.28(3)
C(40)-C(41)	1.42(2)
C(41)-C(42)	1.33(2)
C(41A)-C(42)	1.45(3)
C(43)-C(44A)	1.24(3)
C(43)-C(44)	1.46(3)
C(44)-C(45)	1.30(3)
C(44A)-C(45)	1.44(3)
C(46)-C(47)	1.33(3)
C(46)-C(47A)	1.41(3)
C(47)-C(48)	1.26(3)
C(47A)-C(48)	1.33(3)
B(1)-F(24)	1.29(3)
B(1)-F(1)	1.352(12)

B(1)-F(3)	1.363(19)
B(1)-F(22)	1.36(2)
B(1)-F(23)	1.436(18)
B(1)-F(2)	1.43(3)
B(1)-F(4)	1.50(3)
B(2)-F(37)	1.30(2)
B(2)-F(36)	1.36(2)
B(2)-F(38)	1.37(2)
B(2)-F(6)	1.39(2)
B(2)-F(7)	1.40(2)
B(2)-F(5)	1.415(16)
B(2)-F(8)	1.46(3)
B(3)-F(10)	1.321(19)
B(3)-F(40)	1.36(2)
B(3)-F(41)	1.38(4)
B(3)-F(9)	1.380(16)
B(3)-F(11)	1.39(2)
B(3)-F(12)	1.40(2)
B(3)-F(42)	1.43(3)
C(49)-N(10)	1.55(2)
N(10)-O(1)	1.180(14)
N(10)-O(2)	1.189(15)
C(50)-N(11)	1.50(3)
N(11)-O(4)	1.23(2)
N(11)-O(3)	1.35(2)
C(51)-C(51)#1	1.42(5)
C(51)-N(12)	1.58(3)
N(12)-O(6)	1.19(3)
N(12)-O(5)	1.26(3)

Table S5. Bond angles [deg] for **1**.

N(2)-Pd(1)-N(3)	78.4(3)
N(2)-Pd(1)-C(40)	177.7(5)
N(3)-Pd(1)-C(40)	102.0(4)
N(2)-Pd(1)-C(41)	139.9(6)
N(3)-Pd(1)-C(41)	135.3(5)
C(40)-Pd(1)-C(41)	38.7(6)
N(2)-Pd(1)-C(42)	110.9(3)
N(3)-Pd(1)-C(42)	170.7(3)
C(40)-Pd(1)-C(42)	68.7(4)
C(41)-Pd(1)-C(42)	36.2(6)
N(2)-Pd(1)-C(41A)	146.2(7)
N(3)-Pd(1)-C(41A)	132.5(8)
C(40)-Pd(1)-C(41A)	34.2(7)
C(41)-Pd(1)-C(41A)	29.5(8)
C(42)-Pd(1)-C(41A)	38.8(8)
N(5)-Pd(2)-C(43)	178.3(5)
N(5)-Pd(2)-N(6)	77.2(3)
C(43)-Pd(2)-N(6)	104.1(4)
N(5)-Pd(2)-C(44A)	145.2(7)
C(43)-Pd(2)-C(44A)	33.9(8)
N(6)-Pd(2)-C(44A)	134.6(7)
N(5)-Pd(2)-C(45)	109.5(4)
C(43)-Pd(2)-C(45)	69.1(5)
N(6)-Pd(2)-C(45)	173.2(4)
C(44A)-Pd(2)-C(45)	39.4(8)
N(5)-Pd(2)-C(44)	138.7(7)
C(43)-Pd(2)-C(44)	39.6(7)
N(6)-Pd(2)-C(44)	138.6(7)
C(44A)-Pd(2)-C(44)	28.3(8)
C(45)-Pd(2)-C(44)	34.9(6)
C(47)-Pd(3)-C(48)	35.0(9)
C(47)-Pd(3)-C(47A)	24.9(9)
C(48)-Pd(3)-C(47A)	36.8(7)
C(47)-Pd(3)-N(8)	144.3(10)
C(48)-Pd(3)-N(8)	177.9(5)
C(47A)-Pd(3)-N(8)	141.3(6)
C(47)-Pd(3)-N(9)	137.3(10)
C(48)-Pd(3)-N(9)	103.4(5)
C(47A)-Pd(3)-N(9)	133.5(6)
N(8)-Pd(3)-N(9)	77.7(3)
C(47)-Pd(3)-C(46)	36.5(9)
C(48)-Pd(3)-C(46)	69.4(5)
C(47A)-Pd(3)-C(46)	38.4(7)
N(8)-Pd(3)-C(46)	109.4(4)
N(9)-Pd(3)-C(46)	171.9(4)
C(16)-N(1)-N(2)	109.6(7)
C(16)-N(1)-C(13)	129.4(7)
N(2)-N(1)-C(13)	120.2(6)
C(18)-N(2)-N(1)	103.7(7)
C(18)-N(2)-Pd(1)	113.1(5)
N(1)-N(2)-Pd(1)	140.1(6)
C(23)-N(3)-C(19)	117.8(9)
C(23)-N(3)-Pd(1)	126.9(7)
C(19)-N(3)-Pd(1)	115.3(6)
C(24)-N(4)-N(5)	111.3(7)
C(24)-N(4)-C(14)	131.0(8)
N(5)-N(4)-C(14)	117.7(7)
N(4)-N(5)-C(26)	105.2(7)
N(4)-N(5)-Pd(2)	138.3(5)
C(26)-N(5)-Pd(2)	116.6(6)
C(31)-N(6)-C(27)	120.7(8)
C(31)-N(6)-Pd(2)	125.7(7)
C(27)-N(6)-Pd(2)	113.6(5)
N(8)-N(7)-C(32)	110.3(7)
N(8)-N(7)-C(15)	119.3(6)
C(32)-N(7)-C(15)	129.6(7)
N(7)-N(8)-C(34)	106.6(7)
N(7)-N(8)-Pd(3)	138.1(6)
C(34)-N(8)-Pd(3)	111.6(6)
C(35)-N(9)-C(39)	117.9(10)
C(35)-N(9)-Pd(3)	115.7(6)
C(39)-N(9)-Pd(3)	126.2(8)
C(2)-C(1)-C(6)	119.7(8)
C(2)-C(1)-C(7)	120.6(8)
C(6)-C(1)-C(7)	119.8(7)
C(1)-C(2)-C(3)	118.9(8)
C(1)-C(2)-C(13)	122.4(8)
C(3)-C(2)-C(13)	118.6(7)
C(4)-C(3)-C(2)	120.1(7)
C(4)-C(3)-C(9)	121.4(8)
C(2)-C(3)-C(9)	118.5(8)
C(5)-C(4)-C(3)	121.1(8)
C(5)-C(4)-C(14)	118.0(8)
C(3)-C(4)-C(14)	120.9(8)
C(4)-C(5)-C(6)	119.0(8)
C(4)-C(5)-C(11)	122.2(8)

C(6)-C(5)-C(11)	118.8(8)	C(37)-C(38)-C(39)	117.8(12)
C(5)-C(6)-C(1)	121.2(7)	N(9)-C(39)-C(38)	122.8(13)
C(5)-C(6)-C(15)	120.5(8)	C(41A)-C(40)-C(41)	48.2(14)
C(1)-C(6)-C(15)	118.4(7)	C(41A)-C(40)-Pd(1)	75.8(13)
C(1)-C(7)-C(8)	112.1(7)	C(41)-C(40)-Pd(1)	70.6(8)
C(3)-C(9)-C(10)	111.5(7)	C(42)-C(41)-C(40)	123.2(16)
C(5)-C(11)-C(12)	112.4(8)	C(42)-C(41)-Pd(1)	72.5(9)
N(1)-C(13)-C(2)	109.7(7)	C(40)-C(41)-Pd(1)	70.6(9)
N(4)-C(14)-C(4)	111.9(7)	C(40)-C(41A)-C(42)	125(2)
N(7)-C(15)-C(6)	110.2(6)	C(40)-C(41A)-Pd(1)	70.0(13)
N(1)-C(16)-C(17)	110.3(8)	C(42)-C(41A)-Pd(1)	68.7(11)
C(16)-C(17)-C(18)	103.9(8)	C(41)-C(42)-C(41A)	46.7(12)
N(2)-C(18)-C(17)	112.4(8)	C(41)-C(42)-Pd(1)	71.3(9)
N(2)-C(18)-C(19)	118.2(8)	C(41A)-C(42)-Pd(1)	72.5(12)
C(17)-C(18)-C(19)	129.3(8)	C(44A)-C(43)-C(44)	45.2(14)
C(20)-C(19)-N(3)	121.8(8)	C(44A)-C(43)-Pd(2)	73.5(14)
C(20)-C(19)-C(18)	124.4(8)	C(44)-C(43)-Pd(2)	72.8(11)
N(3)-C(19)-C(18)	113.7(8)	C(45)-C(44)-C(43)	122(2)
C(19)-C(20)-C(21)	119.8(10)	C(45)-C(44)-Pd(2)	70.2(12)
C(22)-C(21)-C(20)	119.2(10)	C(43)-C(44)-Pd(2)	67.5(11)
C(21)-C(22)-C(23)	120.0(9)	C(43)-C(44A)-C(45)	129(2)
N(3)-C(23)-C(22)	121.3(10)	C(43)-C(44A)-Pd(2)	72.5(14)
N(4)-C(24)-C(25)	107.5(9)	C(45)-C(44A)-Pd(2)	70.5(11)
C(24)-C(25)-C(26)	106.8(8)	C(44)-C(45)-C(44A)	45.2(14)
N(5)-C(26)-C(25)	109.3(8)	C(44)-C(45)-Pd(2)	75.0(12)
N(5)-C(26)-C(27)	115.0(8)	C(44A)-C(45)-Pd(2)	70.2(11)
C(25)-C(26)-C(27)	135.4(8)	C(47)-C(46)-C(47A)	38.7(16)
N(6)-C(27)-C(28)	120.2(8)	C(47)-C(46)-Pd(3)	69.6(15)
N(6)-C(27)-C(26)	116.5(7)	C(47A)-C(46)-Pd(3)	69.4(10)
C(28)-C(27)-C(26)	123.2(9)	C(48)-C(47)-C(46)	138(3)
C(29)-C(28)-C(27)	118.8(10)	C(48)-C(47)-Pd(3)	72.9(16)
C(30)-C(29)-C(28)	119.7(9)	C(46)-C(47)-Pd(3)	73.9(15)
C(29)-C(30)-C(31)	120.4(10)	C(48)-C(47A)-C(46)	124(2)
N(6)-C(31)-C(30)	119.8(11)	C(48)-C(47A)-Pd(3)	71.2(11)
N(7)-C(32)-C(33)	109.0(8)	C(46)-C(47A)-Pd(3)	72.1(11)
C(32)-C(33)-C(34)	104.1(9)	C(47)-C(48)-C(47A)	40.8(16)
N(8)-C(34)-C(33)	110.1(8)	C(47)-C(48)-Pd(3)	72.1(15)
N(8)-C(34)-C(35)	119.1(8)	C(47A)-C(48)-Pd(3)	72.0(11)
C(33)-C(34)-C(35)	130.9(9)	F(24)-B(1)-F(1)	111.6(15)
N(9)-C(35)-C(36)	123.6(10)	F(24)-B(1)-F(3)	88.6(15)
N(9)-C(35)-C(34)	113.2(9)	F(1)-B(1)-F(3)	115.7(12)
C(36)-C(35)-C(34)	123.2(10)	F(24)-B(1)-F(22)	99.9(18)
C(37)-C(36)-C(35)	117.6(13)	F(1)-B(1)-F(22)	115.9(13)
C(36)-C(37)-C(38)	120.2(13)	F(3)-B(1)-F(22)	119.6(14)

F(24)-B(1)-F(23)	117.2(15)
F(1)-B(1)-F(23)	106.0(10)
F(3)-B(1)-F(23)	29.0(8)
F(22)-B(1)-F(23)	106.6(13)
F(24)-B(1)-F(2)	119.2(18)
F(1)-B(1)-F(2)	104.1(12)
F(3)-B(1)-F(2)	117.8(15)
F(22)-B(1)-F(2)	19.3(12)
F(23)-B(1)-F(2)	96.9(12)
F(24)-B(1)-F(4)	14.5(16)
F(1)-B(1)-F(4)	106.2(11)
F(3)-B(1)-F(4)	103.0(15)
F(22)-B(1)-F(4)	90.9(15)
F(23)-B(1)-F(4)	131.3(13)
F(2)-B(1)-F(4)	109.5(15)
F(37)-B(2)-F(36)	104.1(17)
F(37)-B(2)-F(38)	103.9(15)
F(36)-B(2)-F(38)	113.9(18)
F(37)-B(2)-F(6)	81.7(15)
F(36)-B(2)-F(6)	29.3(11)
F(38)-B(2)-F(6)	139.0(18)
F(37)-B(2)-F(7)	32.4(10)
F(36)-B(2)-F(7)	134.9(18)
F(38)-B(2)-F(7)	94.6(16)
F(6)-B(2)-F(7)	108.3(15)
F(37)-B(2)-F(5)	127.5(16)
F(36)-B(2)-F(5)	105.2(14)
F(38)-B(2)-F(5)	102.5(14)
F(6)-B(2)-F(5)	105.6(13)
F(7)-B(2)-F(5)	101.4(14)
F(37)-B(2)-F(8)	110.8(15)
F(36)-B(2)-F(8)	80.5(16)
F(38)-B(2)-F(8)	33.6(10)
F(6)-B(2)-F(8)	106.0(17)
F(7)-B(2)-F(8)	118.5(16)
F(5)-B(2)-F(8)	116.3(13)
F(10)-B(3)-F(40)	27.6(10)
F(10)-B(3)-F(41)	73.3(18)
F(40)-B(3)-F(41)	100(2)
F(10)-B(3)-F(9)	116.2(14)
F(40)-B(3)-F(9)	100.6(15)
F(41)-B(3)-F(9)	108.4(18)
F(10)-B(3)-F(11)	103.8(14)
F(40)-B(3)-F(11)	131.4(16)
F(41)-B(3)-F(11)	34.8(17)
F(9)-B(3)-F(11)	108.9(13)
F(10)-B(3)-F(12)	106.7(14)
F(40)-B(3)-F(12)	92.8(14)
F(41)-B(3)-F(12)	137(2)
F(9)-B(3)-F(12)	109.6(12)
F(11)-B(3)-F(12)	111.5(15)
F(10)-B(3)-F(42)	121(2)
F(40)-B(3)-F(42)	116(2)
F(41)-B(3)-F(42)	116(2)
F(9)-B(3)-F(42)	114.0(17)
F(11)-B(3)-F(42)	86.5(19)
F(12)-B(3)-F(42)	25.8(15)
O(1)-N(10)-O(2)	118.3(14)
O(1)-N(10)-C(49)	118.9(13)
O(2)-N(10)-C(49)	120.9(15)
O(4)-N(11)-O(3)	113(2)
O(4)-N(11)-C(50)	126(2)
O(3)-N(11)-C(50)	121(2)
C(51)#1-C(51)-N(12)	140(3)
O(6)-N(12)-O(5)	129(3)
O(6)-N(12)-C(51)	112(3)
O(5)-N(12)-C(51)	119(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1 -y -z

Table S6. Bond lengths [Å] for **2**.

Rh(1)-N(3)	2.117(6)	C(3)-C(9)	1.535(10)
Rh(1)-C(61)	2.132(8)	C(4)-C(5)	1.413(10)
Rh(1)-N(2)	2.133(5)	C(4)-C(14)	1.509(10)
Rh(1)-C(56)	2.137(9)	C(5)-C(6)	1.407(10)
Rh(1)-C(60)	2.141(6)	C(5)-C(11)	1.536(9)
Rh(1)-C(57)	2.149(8)	C(6)-C(15)	1.525(9)
Rh(2)-C(54)	2.107(9)	C(7)-C(8)	1.517(10)
Rh(2)-N(5)	2.110(6)	C(9)-C(10)	1.552(12)
Rh(2)-N(6)	2.128(5)	C(11)-C(12)	1.517(12)
Rh(2)-C(55)	2.130(7)	C(16)-C(17)	1.378(12)
Rh(2)-C(50)	2.146(7)	C(17)-C(18)	1.388(10)
Rh(2)-C(51)	2.166(6)	C(18)-C(19)	1.431(11)
Rh(3)-N(8)	2.120(6)	C(19)-C(20)	1.387(10)
Rh(3)-C(45)	2.124(9)	C(20)-C(21)	1.375(12)
Rh(3)-N(9)	2.127(6)	C(21)-C(22)	1.346(12)
Rh(3)-C(44)	2.130(6)	C(22)-C(23)	1.387(13)
Rh(3)-C(40)	2.145(7)	C(24)-C(25)	1.336(10)
Rh(3)-C(41)	2.157(8)	C(25)-C(26)	1.372(11)
N(1)-C(16)	1.355(9)	C(26)-C(27)	1.477(10)
N(1)-N(2)	1.359(8)	C(27)-C(28)	1.364(10)
N(1)-C(13)	1.467(9)	C(28)-C(29)	1.394(11)
N(2)-C(18)	1.363(10)	C(29)-C(30)	1.373(13)
N(3)-C(23)	1.346(10)	C(30)-C(31)	1.418(10)
N(3)-C(19)	1.372(9)	C(32)-C(33)	1.361(12)
N(4)-C(24)	1.358(9)	C(33)-C(34)	1.392(12)
N(4)-N(5)	1.369(8)	C(34)-C(35)	1.445(10)
N(4)-C(14)	1.487(9)	C(35)-C(36)	1.397(11)
N(5)-C(26)	1.347(8)	C(36)-C(37)	1.379(13)
N(6)-C(31)	1.315(9)	C(37)-C(38)	1.416(13)
N(6)-C(27)	1.345(10)	C(38)-C(39)	1.392(12)
N(7)-C(32)	1.309(10)	C(40)-C(41)	1.405(12)
N(7)-N(8)	1.369(8)	C(40)-C(47)	1.495(12)
N(7)-C(15)	1.477(9)	C(41)-C(42)	1.512(11)
N(8)-C(34)	1.341(9)	C(42)-C(43)	1.550(11)
N(9)-C(39)	1.340(9)	C(43)-C(44)	1.489(13)
N(9)-C(35)	1.371(10)	C(44)-C(45)	1.392(13)
C(1)-C(6)	1.392(9)	C(45)-C(46)	1.519(12)
C(1)-C(2)	1.405(10)	C(46)-C(47)	1.530(11)
C(1)-C(7)	1.513(10)	C(48)-C(49)	1.511(14)
C(2)-C(3)	1.412(11)	C(48)-C(55)	1.553(11)
C(2)-C(13)	1.506(9)	C(49)-C(50)	1.502(12)
C(3)-C(4)	1.389(10)	C(50)-C(51)	1.417(11)
		C(51)-C(52)	1.533(11)
		C(52)-C(53)	1.535(11)

C(53)-C(54)	1.500(11)	N(02)-C(05B)#1	1.49(2)
C(54)-C(55)	1.368(12)	C(05A)-C(05B)	0.72(3)
C(56)-C(57)	1.398(16)	C(05A)-O(06B)#1	1.65(4)
C(56)-C(63)	1.517(15)	C(05A)-O(07B)	1.72(3)
C(57)-C(58)	1.495(14)	O(06A)-O(07B)	0.68(3)
C(58)-C(59)	1.432(14)	O(06A)-O(06B)	1.16(3)
C(59)-C(60)	1.535(12)	O(07A)-O(06B)	1.17(3)
C(60)-C(61)	1.429(13)	O(07A)-C(05B)	1.45(3)
C(61)-C(62)	1.504(13)	O(07A)-O(07B)#1	1.59(3)
C(62)-C(63)	1.498(15)	O(06B)-C(05A)#1	1.65(4)
B(1)-F(3)	1.370(10)	O(06B)-O(07B)	1.69(3)
B(1)-F(1)	1.371(11)	O(07B)-O(07A)#1	1.59(3)
B(1)-F(2)	1.378(11)		
B(1)-F(4)	1.395(11)		
B(2)-F(6)	1.331(14)		
B(2)-F(8)	1.345(15)		
B(2)-F(7)	1.371(11)		
B(2)-F(5)	1.391(13)		
B(3)-F(12A)	1.23(7)		
B(3)-F(11B)	1.24(3)		
B(3)-F(9)	1.25(2)		
B(3)-F(10A)	1.28(3)		
B(3)-F(10B)	1.47(6)		
B(3)-F(11A)	1.49(3)		
B(3)-F(12B)	1.55(4)		
C(01)-N(01)	1.405(15)		
N(01)-O(01)	1.083(13)		
N(01)-O(02)	1.299(15)		
N(03)-O(06)	1.18(3)		
N(03)-C(03A)	1.22(5)		
N(03)-O(05B)	1.27(4)		
N(03)-C(03B)	1.46(4)		
N(03)-O(05A)	1.55(3)		
N(02)-O(06B)	1.39(3)		
N(02)-O(06B)#1	1.39(3)		
N(02)-O(07B)#1	1.394(19)		
N(02)-O(07B)	1.394(19)		
N(02)-O(07A)	1.40(3)		
N(02)-O(07A)#1	1.40(3)		
N(02)-C(05A)	1.46(2)		
N(02)-C(05A)#1	1.46(2)		
N(02)-O(06A)	1.47(2)		
N(02)-O(06A)#1	1.47(2)		
N(02)-C(05B)	1.49(2)		

Table S7. Bond angles [deg] for **2**.

N(3)-Rh(1)-C(61)	91.9(3)
N(3)-Rh(1)-N(2)	78.8(2)
C(61)-Rh(1)-N(2)	156.1(3)
N(3)-Rh(1)-C(56)	161.7(5)
C(61)-Rh(1)-C(56)	81.2(4)
N(2)-Rh(1)-C(56)	100.7(3)
N(3)-Rh(1)-C(60)	94.7(3)
C(61)-Rh(1)-C(60)	39.1(3)
N(2)-Rh(1)-C(60)	162.1(3)
C(56)-Rh(1)-C(60)	90.7(4)
N(3)-Rh(1)-C(57)	160.2(4)
C(61)-Rh(1)-C(57)	96.9(4)
N(2)-Rh(1)-C(57)	99.0(3)
C(56)-Rh(1)-C(57)	38.1(4)
C(60)-Rh(1)-C(57)	81.4(4)
C(54)-Rh(2)-N(5)	157.1(3)
C(54)-Rh(2)-N(6)	94.9(3)
N(5)-Rh(2)-N(6)	78.4(2)
C(54)-Rh(2)-C(55)	37.7(3)
N(5)-Rh(2)-C(55)	162.6(3)
N(6)-Rh(2)-C(55)	93.5(3)
C(54)-Rh(2)-C(50)	97.5(3)
N(5)-Rh(2)-C(50)	98.1(3)
N(6)-Rh(2)-C(50)	153.1(3)
C(55)-Rh(2)-C(50)	82.1(3)
C(54)-Rh(2)-C(51)	81.6(3)
N(5)-Rh(2)-C(51)	100.6(3)
N(6)-Rh(2)-C(51)	168.5(3)
C(55)-Rh(2)-C(51)	90.3(3)
C(50)-Rh(2)-C(51)	38.4(3)
N(8)-Rh(3)-C(45)	164.4(3)
N(8)-Rh(3)-N(9)	78.8(2)
C(45)-Rh(3)-N(9)	95.7(3)
N(8)-Rh(3)-C(44)	155.1(3)
C(45)-Rh(3)-C(44)	38.2(4)
N(9)-Rh(3)-C(44)	92.2(3)
N(8)-Rh(3)-C(40)	98.8(3)
C(45)-Rh(3)-C(40)	81.2(3)
N(9)-Rh(3)-C(40)	159.5(3)
C(44)-Rh(3)-C(40)	97.5(3)
N(8)-Rh(3)-C(41)	101.0(3)
C(45)-Rh(3)-C(41)	88.7(3)
N(9)-Rh(3)-C(41)	162.3(3)
C(44)-Rh(3)-C(41)	80.7(3)
C(40)-Rh(3)-C(41)	38.1(3)
C(16)-N(1)-N(2)	110.9(6)
C(16)-N(1)-C(13)	125.4(6)
N(2)-N(1)-C(13)	123.5(5)
N(1)-N(2)-C(18)	105.5(5)
N(1)-N(2)-Rh(1)	142.5(5)
C(18)-N(2)-Rh(1)	111.9(5)
C(23)-N(3)-C(19)	117.6(7)
C(23)-N(3)-Rh(1)	128.2(5)
C(19)-N(3)-Rh(1)	113.7(5)
C(24)-N(4)-N(5)	109.6(6)
C(24)-N(4)-C(14)	128.0(6)
N(5)-N(4)-C(14)	122.2(6)
C(26)-N(5)-N(4)	104.7(6)
C(26)-N(5)-Rh(2)	113.4(5)
N(4)-N(5)-Rh(2)	141.4(4)
C(31)-N(6)-C(27)	119.0(6)
C(31)-N(6)-Rh(2)	126.4(5)
C(27)-N(6)-Rh(2)	114.1(4)
C(32)-N(7)-N(8)	111.2(6)
C(32)-N(7)-C(15)	125.3(6)
N(8)-N(7)-C(15)	123.4(6)
C(34)-N(8)-N(7)	104.0(6)
C(34)-N(8)-Rh(3)	112.8(5)
N(7)-N(8)-Rh(3)	143.2(5)
C(39)-N(9)-C(35)	119.3(7)
C(39)-N(9)-Rh(3)	127.2(6)
C(35)-N(9)-Rh(3)	113.4(5)
C(6)-C(1)-C(2)	119.5(7)
C(6)-C(1)-C(7)	120.4(6)
C(2)-C(1)-C(7)	120.1(6)
C(1)-C(2)-C(3)	120.1(6)
C(1)-C(2)-C(13)	120.6(7)
C(3)-C(2)-C(13)	119.3(7)
C(4)-C(3)-C(2)	119.8(7)
C(4)-C(3)-C(9)	119.8(7)
C(2)-C(3)-C(9)	120.3(7)
C(3)-C(4)-C(5)	120.7(7)
C(3)-C(4)-C(14)	119.4(7)
C(5)-C(4)-C(14)	119.9(6)
C(6)-C(5)-C(4)	118.7(6)
C(6)-C(5)-C(11)	121.0(6)

C(4)-C(5)-C(11)	120.3(7)	C(39)-C(38)-C(37)	118.8(8)
C(1)-C(6)-C(5)	121.2(6)	N(9)-C(39)-C(38)	122.0(8)
C(1)-C(6)-C(15)	120.5(7)	C(41)-C(40)-C(47)	124.6(8)
C(5)-C(6)-C(15)	118.3(6)	C(41)-C(40)-Rh(3)	71.4(4)
C(1)-C(7)-C(8)	112.6(7)	C(47)-C(40)-Rh(3)	110.8(5)
C(3)-C(9)-C(10)	111.9(7)	C(40)-C(41)-C(42)	123.0(9)
C(12)-C(11)-C(5)	110.8(6)	C(40)-C(41)-Rh(3)	70.5(4)
N(1)-C(13)-C(2)	111.3(5)	C(42)-C(41)-Rh(3)	113.5(5)
N(4)-C(14)-C(4)	110.6(6)	C(41)-C(42)-C(43)	110.7(6)
N(7)-C(15)-C(6)	111.3(5)	C(44)-C(43)-C(42)	112.1(7)
N(1)-C(16)-C(17)	107.6(7)	C(45)-C(44)-C(43)	126.3(8)
C(16)-C(17)-C(18)	105.8(7)	C(45)-C(44)-Rh(3)	70.6(4)
N(2)-C(18)-C(17)	110.2(7)	C(43)-C(44)-Rh(3)	110.8(5)
N(2)-C(18)-C(19)	119.2(6)	C(44)-C(45)-C(46)	126.0(9)
C(17)-C(18)-C(19)	130.5(7)	C(44)-C(45)-Rh(3)	71.2(5)
N(3)-C(19)-C(20)	121.6(7)	C(46)-C(45)-Rh(3)	113.7(5)
N(3)-C(19)-C(18)	115.9(6)	C(45)-C(46)-C(47)	112.8(7)
C(20)-C(19)-C(18)	122.5(7)	C(40)-C(47)-C(46)	113.2(7)
C(21)-C(20)-C(19)	118.4(8)	C(49)-C(48)-C(55)	111.2(7)
C(22)-C(21)-C(20)	121.0(8)	C(50)-C(49)-C(48)	114.7(7)
C(21)-C(22)-C(23)	118.8(9)	C(51)-C(50)-C(49)	125.2(8)
N(3)-C(23)-C(22)	122.5(8)	C(51)-C(50)-Rh(2)	71.6(4)
C(25)-C(24)-N(4)	108.4(7)	C(49)-C(50)-Rh(2)	109.3(6)
C(24)-C(25)-C(26)	106.3(7)	C(50)-C(51)-C(52)	121.6(8)
N(5)-C(26)-C(25)	111.0(6)	C(50)-C(51)-Rh(2)	70.0(4)
N(5)-C(26)-C(27)	117.6(7)	C(52)-C(51)-Rh(2)	111.6(5)
C(25)-C(26)-C(27)	131.4(7)	C(51)-C(52)-C(53)	111.7(6)
N(6)-C(27)-C(28)	122.7(7)	C(54)-C(53)-C(52)	111.9(7)
N(6)-C(27)-C(26)	115.4(6)	C(55)-C(54)-C(53)	127.7(7)
C(28)-C(27)-C(26)	121.8(8)	C(55)-C(54)-Rh(2)	72.1(5)
C(27)-C(28)-C(29)	118.4(8)	C(53)-C(54)-Rh(2)	111.0(5)
C(30)-C(29)-C(28)	120.1(7)	C(54)-C(55)-C(48)	122.7(7)
C(29)-C(30)-C(31)	117.2(8)	C(54)-C(55)-Rh(2)	70.3(5)
N(6)-C(31)-C(30)	122.5(8)	C(48)-C(55)-Rh(2)	112.8(5)
N(7)-C(32)-C(33)	109.5(7)	C(57)-C(56)-C(63)	123.1(12)
C(32)-C(33)-C(34)	103.9(7)	C(57)-C(56)-Rh(1)	71.4(5)
N(8)-C(34)-C(33)	111.4(7)	C(63)-C(56)-Rh(1)	113.8(7)
N(8)-C(34)-C(35)	119.3(7)	C(56)-C(57)-C(58)	123.0(11)
C(33)-C(34)-C(35)	129.3(7)	C(56)-C(57)-Rh(1)	70.5(5)
N(9)-C(35)-C(36)	121.6(7)	C(58)-C(57)-Rh(1)	109.3(7)
N(9)-C(35)-C(34)	115.6(7)	C(59)-C(58)-C(57)	117.8(9)
C(36)-C(35)-C(34)	122.8(8)	C(58)-C(59)-C(60)	113.6(8)
C(37)-C(36)-C(35)	119.0(9)	C(61)-C(60)-C(59)	123.0(9)
C(36)-C(37)-C(38)	119.2(8)	C(61)-C(60)-Rh(1)	70.1(4)

C(59)-C(60)-Rh(1)	112.1(6)
C(60)-C(61)-C(62)	124.4(9)
C(60)-C(61)-Rh(1)	70.8(4)
C(62)-C(61)-Rh(1)	110.7(6)
C(63)-C(62)-C(61)	115.1(9)
C(62)-C(63)-C(56)	112.3(9)
F(3)-B(1)-F(1)	111.7(8)
F(3)-B(1)-F(2)	107.7(7)
F(1)-B(1)-F(2)	111.1(8)
F(3)-B(1)-F(4)	110.3(8)
F(1)-B(1)-F(4)	108.6(7)
F(2)-B(1)-F(4)	107.4(8)
F(6)-B(2)-F(8)	106.3(11)
F(6)-B(2)-F(7)	112.8(11)
F(8)-B(2)-F(7)	107.4(10)
F(6)-B(2)-F(5)	110.1(9)
F(8)-B(2)-F(5)	110.2(11)
F(7)-B(2)-F(5)	110.0(9)
F(12A)-B(3)-F(11B)	51(3)
F(12A)-B(3)-F(9)	128(4)
F(11B)-B(3)-F(9)	102(3)
F(12A)-B(3)-F(10A)	112(4)
F(11B)-B(3)-F(10A)	158(3)
F(9)-B(3)-F(10A)	99.5(17)
F(12A)-B(3)-F(10B)	123(4)
F(11B)-B(3)-F(10B)	132(3)
F(9)-B(3)-F(10B)	108(2)
F(10A)-B(3)-F(10B)	41(2)
F(12A)-B(3)-F(11A)	93(4)
F(11B)-B(3)-F(11A)	64.7(17)
F(9)-B(3)-F(11A)	117(2)
F(10A)-B(3)-F(11A)	108(2)
F(10B)-B(3)-F(11A)	69(2)
F(12A)-B(3)-F(12B)	46(3)
F(11B)-B(3)-F(12B)	95(2)
F(9)-B(3)-F(12B)	137.4(17)
F(10A)-B(3)-F(12B)	65.5(18)
F(10B)-B(3)-F(12B)	87(3)
F(11A)-B(3)-F(12B)	106(2)
O(01)-N(01)-O(02)	117.4(14)
O(01)-N(01)-C(01)	126.0(17)
O(02)-N(01)-C(01)	116.1(13)
O(06)-N(03)-C(03A)	153(4)
O(06)-N(03)-O(05B)	102(3)
C(03A)-N(03)-O(05B)	57(3)
O(06)-N(03)-C(03B)	154(3)
C(03A)-N(03)-C(03B)	51(3)
O(05B)-N(03)-C(03B)	105(4)
O(06)-N(03)-O(05A)	91(2)
C(03A)-N(03)-O(05A)	114(4)
O(05B)-N(03)-O(05A)	162(3)
C(03B)-N(03)-O(05A)	63(2)
O(06B)-N(02)-O(06B)#1	180.0(19)
O(06B)-N(02)-O(07B)#1	105.2(14)
O(06B)#1-N(02)-O(07B)#1	74.8(14)
O(06B)-N(02)-O(07B)	74.8(14)
O(06B)#1-N(02)-O(07B)	105.2(14)
O(07B)#1-N(02)-O(07B)	180(2)
O(06B)-N(02)-O(07A)	49.6(14)
O(06B)#1-N(02)-O(07A)	130.4(14)
O(07B)#1-N(02)-O(07A)	69.2(14)
O(07B)-N(02)-O(07A)	110.8(14)
O(06B)-N(02)-O(07A)#1	130.4(14)
O(06B)#1-N(02)-O(07A)#1	49.6(14)
O(07B)#1-N(02)-O(07A)#1	110.8(14)
O(07B)-N(02)-O(07A)#1	69.2(14)
O(07A)-N(02)-O(07A)#1	180.0(17)
O(06B)-N(02)-C(05A)	109.4(14)
O(06B)#1-N(02)-C(05A)	70.6(14)
O(07B)#1-N(02)-C(05A)	105.9(13)
O(07B)-N(02)-C(05A)	74.1(13)
O(07A)-N(02)-C(05A)	87.6(15)
O(07A)#1-N(02)-C(05A)	92.4(15)
O(06B)-N(02)-C(05A)#1	70.6(14)
O(06B)#1-N(02)-C(05A)#1	109.4(14)
O(07B)#1-N(02)-C(05A)#1	74.1(13)
O(07B)-N(02)-C(05A)#1	105.9(13)
O(07A)-N(02)-C(05A)#1	92.4(15)
O(07A)#1-N(02)-C(05A)#1	87.6(14)
C(05A)-N(02)-C(05A)#1	180(2)
O(06B)-N(02)-O(06A)	47.9(14)
O(06B)#1-N(02)-O(06A)	132.1(14)
O(07B)#1-N(02)-O(06A)	152.6(11)
O(07B)-N(02)-O(06A)	27.4(11)
O(07A)-N(02)-O(06A)	90.3(15)
O(07A)#1-N(02)-O(06A)	89.7(15)
C(05A)-N(02)-O(06A)	90.5(13)
C(05A)#1-N(02)-O(06A)	89.5(13)

O(06B)-N(02)-O(06A)#1	132.1(14)
O(06B)#1-N(02)-O(06A)#1	47.9(14)
O(07B)#1-N(02)-O(06A)#1	27.4(11)
O(07B)-N(02)-O(06A)#1	152.6(11)
O(07A)-N(02)-O(06A)#1	89.7(15)
O(07A)#1-N(02)-O(06A)#1	90.3(15)
C(05A)-N(02)-O(06A)#1	89.5(13)
C(05A)#1-N(02)-O(06A)#1	90.5(13)
O(06A)-N(02)-O(06A)#1	180.000(4)
O(06B)-N(02)-C(05B)	92.3(14)
O(06B)#1-N(02)-C(05B)	87.7(14)
O(07B)#1-N(02)-C(05B)	90.0(12)
O(07B)-N(02)-C(05B)	90.0(12)
O(07A)-N(02)-C(05B)	60.0(14)
O(07A)#1-N(02)-C(05B)	120.0(14)
C(05A)-N(02)-C(05B)	28.0(11)
C(05A)#1-N(02)-C(05B)	152.0(11)
O(06A)-N(02)-C(05B)	95.2(13)
O(06A)#1-N(02)-C(05B)	84.8(13)
O(06B)-N(02)-C(05B)#1	87.7(14)
O(06B)#1-N(02)-C(05B)#1	92.3(14)
O(07B)#1-N(02)-C(05B)#1	90.0(12)
O(07B)-N(02)-C(05B)#1	90.0(12)
O(07A)-N(02)-C(05B)#1	120.0(14)
O(07A)#1-N(02)-C(05B)#1	60.0(14)
C(05A)-N(02)-C(05B)#1	152.0(11)
C(05A)#1-N(02)-C(05B)#1	28.0(11)
O(06A)-N(02)-C(05B)#1	84.8(13)
O(06A)#1-N(02)-C(05B)#1	95.2(13)
C(05B)-N(02)-C(05B)#1	180(2)
C(05B)-C(05A)-N(02)	78(3)
C(05B)-C(05A)-O(06B)#1	109(3)
N(02)-C(05A)-O(06B)#1	52.6(12)
C(05B)-C(05A)-O(07B)	106(3)
N(02)-C(05A)-O(07B)	51.2(10)
O(06B)#1-C(05A)-O(07B)	81.9(15)
O(07B)-O(06A)-O(06B)	131(4)
O(07B)-O(06A)-N(02)	70(3)
O(06B)-O(06A)-N(02)	62.4(18)
O(06B)-O(07A)-N(02)	64.5(19)
O(06B)-O(07A)-C(05B)	104(2)
N(02)-O(07A)-C(05B)	63.0(15)
O(06B)-O(07A)-O(07B)#1	105(2)
N(02)-O(07A)-O(07B)#1	55.1(12)
C(05B)-O(07A)-O(07B)#1	84.3(18)
C(05A)-C(05B)-O(07A)	130(3)
C(05A)-C(05B)-N(02)	74(3)
O(07A)-C(05B)-N(02)	57.0(13)
O(06A)-O(06B)-O(07A)	122(3)
O(06A)-O(06B)-N(02)	69.7(19)
O(07A)-O(06B)-N(02)	65.9(19)
O(06A)-O(06B)-C(05A)#1	93(2)
O(07A)-O(06B)-C(05A)#1	93(2)
N(02)-O(06B)-C(05A)#1	56.8(13)
O(06A)-O(06B)-O(07B)	17.6(15)
O(07A)-O(06B)-O(07B)	106(2)
N(02)-O(06B)-O(07B)	52.8(11)
C(05A)#1-O(06B)-O(07B)	86.2(17)
O(06A)-O(07B)-N(02)	82(3)
O(06A)-O(07B)-O(07A)#1	121(3)
N(02)-O(07B)-O(07A)#1	55.7(12)
O(06A)-O(07B)-O(06B)	31(3)
N(02)-O(07B)-O(06B)	52.4(11)
O(07A)#1-O(07B)-O(06B)	101.1(17)
O(06A)-O(07B)-C(05A)	113(3)
N(02)-O(07B)-C(05A)	54.8(10)
O(07A)#1-O(07B)-C(05A)	77.2(15)
O(06B)-O(07B)-C(05A) 8	6.0(16)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z