Supporting Information

Unusual Ar-H/Rh-H J_{HH} NMR Coupling in Complexes of Rhodium(III): Experimental Evidence and Theoretical Support for an η^1-Arene Structure

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I. Parameters for 2D NMR experiments performed on **3a-c.**

Homonuclear decoupling experiment for 3b. Homonuclear decoupling experiments were performed on a CD_2Cl_2 solution of **3b** on a Bruker DMX-500 MHz spectrometer using the pulse program *zg0hd*. Spectra were acquired in 8 scans with a relaxation delay of 200 msec. The observation pulse (P1) was calibrated to the $(\pi/4)_x$ pulse length, 7.11 μsec. The decoupler power was set to 34.00 dB. Due to the constraints of the pulse program, the acquisition window has a maximum width of 20 ppm, which is not wide enough to simultaneously visualize both the rhodium hydride (H_b, -21.00 ppm) and the preagostic aryl proton (H_a, 8.79 ppm). In a first experiment, the decoupler was set to irradiate H_b (O2 = -21.00 ppm) with the observation window centered to allow visualization of this resonance (O1 = -15.05 ppm, SW = 19.95 ppm). The resonance for H_b was observed to null. In a second experiment, the position and power of the decoupling pulse were unchanged (O2 = -21.00 ppm, PL24 = 34 dB), but the observation window was shifted to allow for observation of H_a at 8.79 ppm (O1 = 2.03 ppm, SW = 19.95 ppm). In this experiment, H_a was observed to collapse from a doublet ($J_{H\text{-}H}$ = 3.1 Hz) to a sharp singlet. No other ligand resonances were affected by the decoupling pulse. Without changing any other parameters, a second set of experiments was performed with the decoupling pulse centered at H_a (O2 = 8.79 ppm). The resonance for H_a was observed to null and the resonance for H_b collapsed from a doublet of doublets ($J_{H\text{-}H}$ = 3.1 Hz, $^1J_{Rh\text{-}H}$ = 22.1 Hz) to a clean doublet ($^1J_{Rh\text{-}H}$ = 22.1 Hz).

2D TOCSY spectrum of 3b. A 2D TOCSY spectrum was acquired at 23.0 °C on a Bruker DRX-500 MHz spectrometer using the pulse program *mlevtp.ucb.* The temperature was maintained throughout the experiment using the Bruker *edte* temperature control software. The $(\pi/2)_x$ pulse length was calibrated and found to be 14.50 μsec. Based on independent measurements of the relevant T_1 relaxation times (*vide infra*), a mixing time of 1.0 seconds and a recycle delay of 1.5 seconds were used. Data were centered at O1 = -7.48 ppm and spread over a sweep width of 34.96 ppm. The spectrum was acquired in 2 scans with 16 dummy scans in 2048 increments (F1) with 2048 data points (F2). The data

were subjected to Fourier transformation, and the resulting base line was corrected by applying the Bruker *abs* routine to both dimensions. Data were further corrected by symmeterization using Bruker's *sym* command.

2D ^{1}H-^{13}C HMQC spectrum of 3b. A 2D HMQC spectrum was acquired at 22.5 °C on a Bruker DRX-500 MHz spectrometer using the pulse program *invbtp*. The temperature was controlled using the Bruker *edte* temperature control software. The $(\pi/2)_x$ pulse length was calibrated and found to be 14.50 μsec. Data were centered at O1 = -7.48 ppm and spread over a sweep width of 34.96 ppm. The spectrum was acquired in 4 scans with 8 dummy scans in 2048 increments (F1) with 1024 data points (F2). The data were subjected to Fourier transformation, and the resulting base line was corrected by applying the Bruker *abs* routine to both dimensions.

T_1 Minimum Measurements for 3a. The minimum T_1 relaxation times were determined for the aryl proton (H_a) and rhodium hydride (H_b) resonances for **3a** using variable temperature studies on a Bruker DRX-500 spectrometer. The temperature was controlled using the Bruker *edte* temperature control software and was varied from 300 K to 213 K. Temperatures were calibrated with an external methanol standard. T_1 relaxation times for each resonance were obtained every 20 K using the pulse program *quickt1*. The T_1 values obtained by this method were checked by performing a complete inversion recovery sequence for each resonance at 300 K and 238 K, using the Bruker pulse program *t1ircp*. The inversion recovery data were fit with an exponential function using the *autot1* fitting program in Bruker's XWIN-NMR data processing system. These values were found to be in excellent agreement with those obtained by the *quickt1* method. The total variable temperature T_1 data sets were fit to polynomial functions using Microsoft Excel, yielding T_1 minimum values of 962 msec at 240 K for H_a and 301 msec at 238 K for H_b.

1D NOE Difference Spectra of 3b. A difference NOE experiment was acquired for **3b** in d_8-toluene solution at 22.7 °C on a Bruker DRX-500 MHz spectrometer using the pulse program *zg0h1pr*. The temperature was maintained throughout the experiment using the Bruker *edte* temperature control

software. The $(\pi/2)_x$ pulse length was calibrated and found to be 14.25 μsec. Prior to performing the difference NOE experiment, T_1 relaxation times were found to be 1.73 seconds and 648 milliseconds, respectively at this temperature and field strength. Based on this information, the relaxation delay for the difference NOE experiment (D1) was set to 8.6 seconds. The presaturation power level was set to 70 dB. A control experiment was performed with the saturation frequency set to the middle of the spectrum (O2 = -7.1 ppm). In this experiment, the spectrum appeared entirely unperturbed. Two experiments were conducted after the control experiment: one with saturation of the H_b resonance (O2 = -21.00 ppm) and one with saturation of H_a resonance (O2 = 8.79 ppm). Difference spectra were calculated between each saturation experiment and the control experiment. Although the difference spectra showed NOE between H_a and the ligand resonances and between H_b and the resonances, no H_a-H_b NOE was observed in either difference spectrum.

2D NOESY spectrum of 3a. A gradient 2D NOESY spectrum of **3a** was acquired in CD_2Cl_2 at 22.3 °C on a Bruker DRX-500 MHz spectrometer using a broad band (non-gradient) probe. The temperature was maintained throughout the experiment using the Bruker *edte* temperature control software. Homospoil gradients were established using the built-in Bruker BSMS shim spoils. The pulse program *noesyhstp* was used to generate a phase-sensitive spectrum with TPPI phase-cycling. The $(\pi/2)_x$ pulse length was calibrated and found to be 14.5 μsec. Based on previously measured T_1s, the data were collected with a mixing time of 1.0 seconds and a recycle delay of 1.5 seconds. Data were centered at O1 = -5.85 ppm and spread over a sweep width of 32.67 ppm. Positive and negative sine gradients of 1 ms duration and strength of 1.2 kHz were employed with the gradient recovery being part of the mixing time. The spectrum was acquired in 2 scans with 4 dummy scans in 1024 increments (F1) with 16,384 data points (F2). Zero-filling to 2048 x 16,384 and squared cosine multiplication of both dimensions were applied to the data prior to Fourier transformation. The resulting base line was corrected by applying the Bruker *abs* routine to both dimensions.

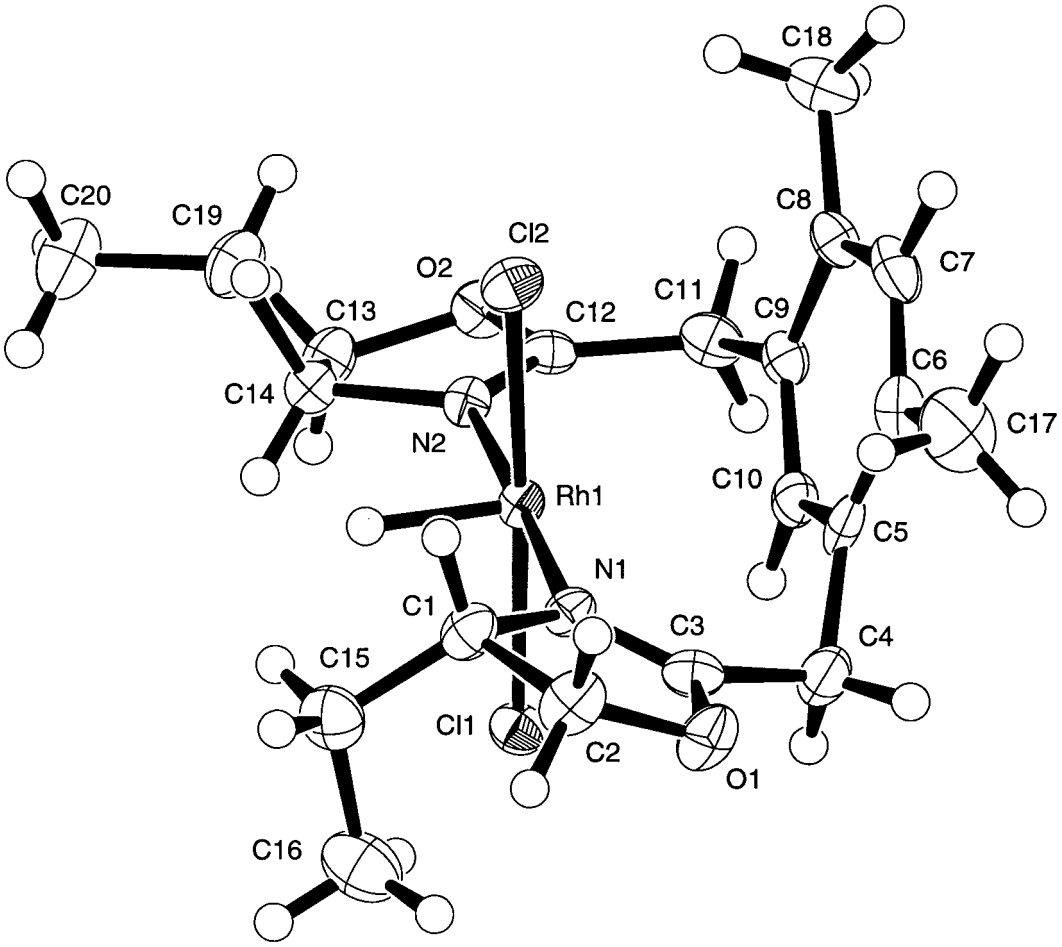

Figure 1. ORTEP diagram of **3a** showing atom numbering scheme. Thermal ellipsoids are shown at 50% probability.

Table 1: Atomic Coordinates and B*iso*/B*eq* for **3a**.

atom	x	y	z	B(eq)
Rh(1)	0.17720(2)	0.21656(2)	0.25650(2)	1.483(5)
Cl(1)	-0.00442(6)	0.21649(8)	0.31867(5)	1.99(2)
Cl(2)	0.35352(6)	0.21043(8)	0.18779(5)	2.20(2)
O(1)	0.0617(2)	0.4402(2)	0.0637(2)	2.52(6)
O(2)	0.2713(2)	0.0797(2)	0.5192(1)	2.09(5)
N(1)	0.1228(2)	0.3009(2)	0.1432(2)	1.67(6)
N(2)	0.2263(2)	0.1286(2)	0.3708(2)	1.52(6)
C(1)	0.1119(3)	0.2633(3)	0.0429(2)	2.16(8)
C(2)	0.0826(3)	0.3636(3)	-0.0109(2)	2.62(9)
C(3)	0.0931(3)	0.3959(3)	0.1467(2)	2.05(8)
C(4)	0.0938(3)	0.4616(3)	0.2351(3)	2.48(9)
C(5)	0.2011(3)	0.4420(3)	0.2900(2)	2.09(8)
C(6)	0.3023(3)	0.4806(2)	0.2582(3)	2.36(8)
C(7)	0.3984(3)	0.4481(3)	0.3048(3)	2.47(9)
C(8)	0.3989(3)	0.3762(3)	0.3791(2)	1.92(8)
C(9)	0.2961(3)	0.3413(3)	0.4124(2)	1.76(8)
C(10)	0.1986(3)	0.3771(3)	0.3694(2)	1.88(8)
C(11)	0.2859(3)	0.2602(3)	0.4899(2)	2.24(8)
C(12)	0.2605(3)	0.1553(3)	0.4541(2)	1.67(8)
C(13)	0.2203(3)	-0.0116(3)	0.4765(2)	2.34(9)
C(14)	0.2155(3)	0.0139(3)	0.3695(2)	1.81(8)
C(15)	0.0296(3)	0.1764(3)	0.0305(3)	2.83(9)
C(16)	-0.0852(3)	0.2016(4)	0.0653(3)	3.7(1)
C(17)	0.3097(4)	0.5527(3)	0.1729(3)	4.0(1)
C(18)	0.5064(3)	0.3376(3)	0.4189(2)	2.75(9)
C(19)	0.3078(3)	-0.0341(3)	0.3106(2)	2.58(9)
C(20)	0.2913(3)	-0.1499(3)	0.2954(3)	3.20(9)
H(1)	0.1827	0.2402	0.0216	2.5961
H(2)	0.0181	0.354	-0.0493	3.1506
H(3)	0.1428	0.3846	-0.0505	3.1506
H(4)	0.0896	0.5323	0.2176	2.9729
H(5)	0.032	0.4443	0.2743	2.9729
H(6)	0.4674	0.4764	0.2849	2.9598
H(7)	0.1288	0.3567	0.3951	2.2518

Table 1: Atomic Coordinates and B*iso*/B*eq* for **3a** (cont.).

atom	x	y	z	B(eq)
H(8)	0.3542	0.2574	0.5239	2.6872
H(9)	0.2281	0.2804	0.5323	2.6872
H(10)	0.2645	-0.0711	0.4876	2.8135
H(11)	0.1478	-0.0225	0.5015	2.8135
H(12)	0.1452	-0.0052	0.344	2.1757
H(13)	0.0253	0.1599	-0.0358	3.3922
H(14)	0.0559	0.1182	0.0651	3.3922
H(15)	-0.1357	0.1505	0.0431	4.3932
H(16)	-0.0856	0.2029	0.1333	4.3932
H(17)	-0.1068	0.2672	0.0413	4.3932
H(18)	0.3832	0.5791	0.168	4.8215
H(19)	0.2917	0.516	0.1161	4.8215
H(20)	0.2591	0.6082	0.1811	4.8215
H(21)	0.5648	0.3827	0.4003	3.3023
H(22)	0.502	0.3353	0.4868	3.3023
H(23)	0.5207	0.2703	0.3948	3.3023
H(24)	0.31	-0.0012	0.2497	3.0996
H(25)	0.3764	-0.0235	0.3428	3.0996
H(26)	0.224	-0.1613	0.2614	3.8419
H(27)	0.3518	-0.1767	0.2595	3.8419
H(28)	0.2878	-0.1835	0.3558	3.8419
H(29)	0.148(3)	0.123(2)	0.206(2)	2.6315

Table 2: Anisotropic Displacement Parameters for **3a**.

atom	U11	U22	U33	U12	U13	U23
Rh(1)	0.0215(1)	0.0187(1)	0.0162(1)	0.0017(1)	0.0000(1)	0.0000(1)
Cl(1)	0.0230(4)	0.0288(5)	0.0236(4)	-0.0024(5)	0.0020(3)	0.0006(5)
Cl(2)	0.0267(5)	0.0328(5)	0.0242(4)	0.0039(5)	0.0060(3)	0.0003(5)
O(1)	0.046(2)	0.026(2)	0.024(1)	0.012(1)	-0.007(1)	0.006(1)
O(2)	0.030(1)	0.028(2)	0.021(1)	0.001(1)	-0.004(1)	0.008(1)
N(1)	0.023(1)	0.022(2)	0.019(1)	0.004(1)	0.000(1)	0.002(1)
N(2)	0.022(2)	0.019(2)	0.017(1)	0.000(1)	0.005(1)	0.001(1)
C(1)	0.031(2)	0.029(2)	0.022(2)	0.006(2)	0.000(2)	-0.002(2)
C(2)	0.043(2)	0.036(2)	0.020(2)	0.010(2)	-0.002(2)	0.002(2)
C(3)	0.021(2)	0.033(2)	0.024(2)	0.001(2)	-0.003(2)	0.003(2)
C(4)	0.037(2)	0.025(2)	0.032(2)	0.008(2)	-0.005(2)	-0.005(2)
C(5)	0.038(2)	0.014(2)	0.028(2)	0.008(2)	0.000(2)	-0.005(1)
C(6)	0.040(2)	0.022(2)	0.028(2)	-0.003(2)	0.000(2)	-0.002(2)
C(7)	0.034(2)	0.029(2)	0.031(2)	-0.015(2)	0.007(2)	-0.007(2)
C(8)	0.027(2)	0.026(2)	0.020(2)	-0.006(2)	-0.004(2)	-0.004(2)
C(9)	0.026(2)	0.024(2)	0.017(2)	-0.003(2)	-0.001(1)	-0.005(2)
C(10)	0.027(2)	0.022(2)	0.022(2)	0.000(2)	0.001(2)	-0.006(2)
C(11)	0.026(2)	0.036(2)	0.023(2)	-0.003(2)	-0.002(1)	0.002(2)
C(12)	0.016(2)	0.026(2)	0.022(2)	-0.001(2)	0.003(2)	0.003(2)
C(13)	0.036(2)	0.021(2)	0.032(2)	0.004(2)	0.001(2)	0.004(2)
C(14)	0.024(2)	0.023(2)	0.021(2)	0.001(2)	0.000(2)	0.001(2)
C(15)	0.039(2)	0.038(2)	0.030(2)	-0.001(2)	-0.008(2)	0.000(2)
C(16)	0.042(2)	0.062(3)	0.035(2)	-0.009(2)	-0.003(2)	0.000(2)
C(17)	0.063(3)	0.042(3)	0.048(2)	-0.010(3)	-0.007(2)	0.020(2)
C(18)	0.026(2)	0.050(3)	0.028(2)	-0.006(2)	-0.001(2)	0.001(2)
C(19)	0.041(3)	0.025(2)	0.031(2)	0.005(2)	0.006(2)	0.005(2)
C(20)	0.058(3)	0.030(2)	0.034(2)	0.004(2)	0.015(2)	0.004(2)

Table 3: Bond lengths (Å) for **3a**.

atom	atom	distance	atom	atom	distance
Rh1	Cl1	2.3509(8)	C4	C5	1.523(5)
Rh1	Cl2	2.3291(8)	C5	C6	1.388(5)
Rh1	N1	2.029(3)	C5	C10	1.391(4)
Rh1	N2	2.046(3)	C6	C7	1.392(5)
O1	C2	1.460(4)	C6	C17	1.516(5)
O1	C3	1.347(4)	C7	C8	1.393(5)
O2	C12	1.343(4)	C8	C9	1.396(5)
O2	C13	1.459(4)	C8	C18	1.493(5)
N1	C1	1.487(4)	C9	C10	1.397(5)
N1	C3	1.283(4)	C9	C11	1.513(5)
N2	C12	1.281(4)	C11	C12	1.480(5)
N2	C14	1.491(4)	C13	C14	1.530(4)
C1	C2	1.542(5)	C14	C19	1.515(5)
C1	C15	1.509(5)	C15	C16	1.499(5)
C3	C4	1.499(5)	C19	C20	1.527(5)
Rh1	H29	1.45(3)	C16	H15	0.95
C1	H1	0.95	C16	H16	0.95
C2	H2	0.95	C16	H17	0.95
C2	H3	0.95	C17	H18	0.95
C4	H4	0.95	C17	H19	0.95
C4	H5	0.95	C17	H20	0.95
C7	H6	0.95	C18	H21	0.95
C10	H7	0.95	C18	H22	0.95
C11	H8	0.95	C18	H23	0.95
C11	H9	0.95	C19	H24	0.95
C13	H10	0.95	C19	H25	0.95
C13	H11	0.95	C20	H26	0.95
C14	H12	0.95	C20	H27	0.95
C15	H13	0.95	C20	H28	0.95
C15	H14	0.95			

Table 4: Bond angles (Å) for **3a**.

atom	atom	atom	angle	atom	atom	atom	angle
Cl1	Rh1	Cl2	176.68(3)	C4	C5	C10	118.9(3)
Cl1	Rh1	N1	89.31(7)	C6	C5	C10	119.4(3)
Cl1	Rh1	N2	88.89(7)	C5	C6	C7	118.0(3)
Cl2	Rh1	N1	89.51(7)	C5	C6	C17	121.7(3)
Cl2	Rh1	N2	92.22(7)	C7	C6	C17	120.3(3)
N1	Rh1	N2	177.8(1)	C6	C7	C8	123.6(3)
C2	O1	C3	105.9(3)	C7	C8	C9	117.4(3)
C12	O2	C13	105.9(2)	C7	C8	C18	120.3(3)
Rh1	N1	C1	125.8(2)	C9	C8	C18	122.4(3)
Rh1	N1	C3	125.2(2)	C8	C9	C10	119.6(3)
C1	N1	C3	109.0(3)	C8	C9	C11	122.3(3)
Rh1	N2	C12	130.5(3)	C10	C9	C11	118.0(3)
Rh1	N2	C14	121.4(2)	C5	C10	C9	121.6(3)
C12	N2	C14	107.9(3)	C9	C11	C12	114.4(3)
N1	C1	C2	101.7(3)	O2	C12	N2	116.6(3)
N1	C1	C15	114.2(3)	O2	C12	C11	114.9(3)
C2	C1	C15	115.0(3)	N2	C12	C11	128.4(3)
O1	C2	C1	105.4(2)	O2	C13	C14	103.9(3)
O1	C3	N1	117.1(3)	N2	C14	C13	101.5(3)
O1	C3	C4	117.9(3)	N2	C14	C19	110.6(3)
N1	C3	C4	125.0(3)	C13	C14	C19	114.4(3)
C3	C4	C5	108.9(3)	C14	C15	C16	113.9(3)
C4	C5	C6	121.5(3)	C14	C19	C20	112.5(3)
Cl1	Rh1	H29	87(1)	O2	C13	H10	110.87
Cl2	Rh1	H29	90(1)	O2	C13	H11	110.87
N1	Rh1	H29	89(1)	C14	C13	H10	110.85

Table 4: Bond angles (Å) for **3a** (cont.).

atom	atom	atom	angle	atom	atom	atom	angle
N2	Rh1	H29	89(1)	C14	C13	H11	110.85
N1	C1	H1	108.52	H10	C13	H11	109.46
C2	C1	H1	108.53	N2	C14	H12	110
C15	C1	H1	108.52	C13	C14	H12	110.01
O1	C2	H2	110.48	C19	C14	H12	110
O1	C2	H3	110.47	C1	C15	H13	108.36
C1	C2	H2	110.5	C1	C15	H14	108.36
C1	C2	H3	110.5	C16	C15	H13	108.36
H2	C2	H3	109.46	C16	C15	H14	108.35
C3	C4	H4	109.6	H13	C15	H14	109.46
C3	C4	H5	109.61	C15	C16	H15	109.47
C5	C4	H4	109.6	C15	C16	H16	109.47
C5	C4	H5	109.61	C15	C16	H17	109.46
H4	C4	H5	109.46	H15	C16	H16	109.48
C6	C7	H6	118.18	H15	C16	H17	109.47
C8	C7	H6	118.18	H16	C16	H17	109.48
C5	C10	H7	119.19	C6	C17	H18	109.47
C9	C10	H7	119.19	C6	C17	H19	109.48
C9	C11	H8	108.23	C6	C17	H20	109.47
C9	C11	H9	108.24	H18	C17	H19	109.47
C12	C11	H8	108.21	H18	C17	H20	109.47
C12	C11	H9	108.23	H19	C17	H20	109.48
H8	C11	H9	109.46	C8	C18	H21	109.48

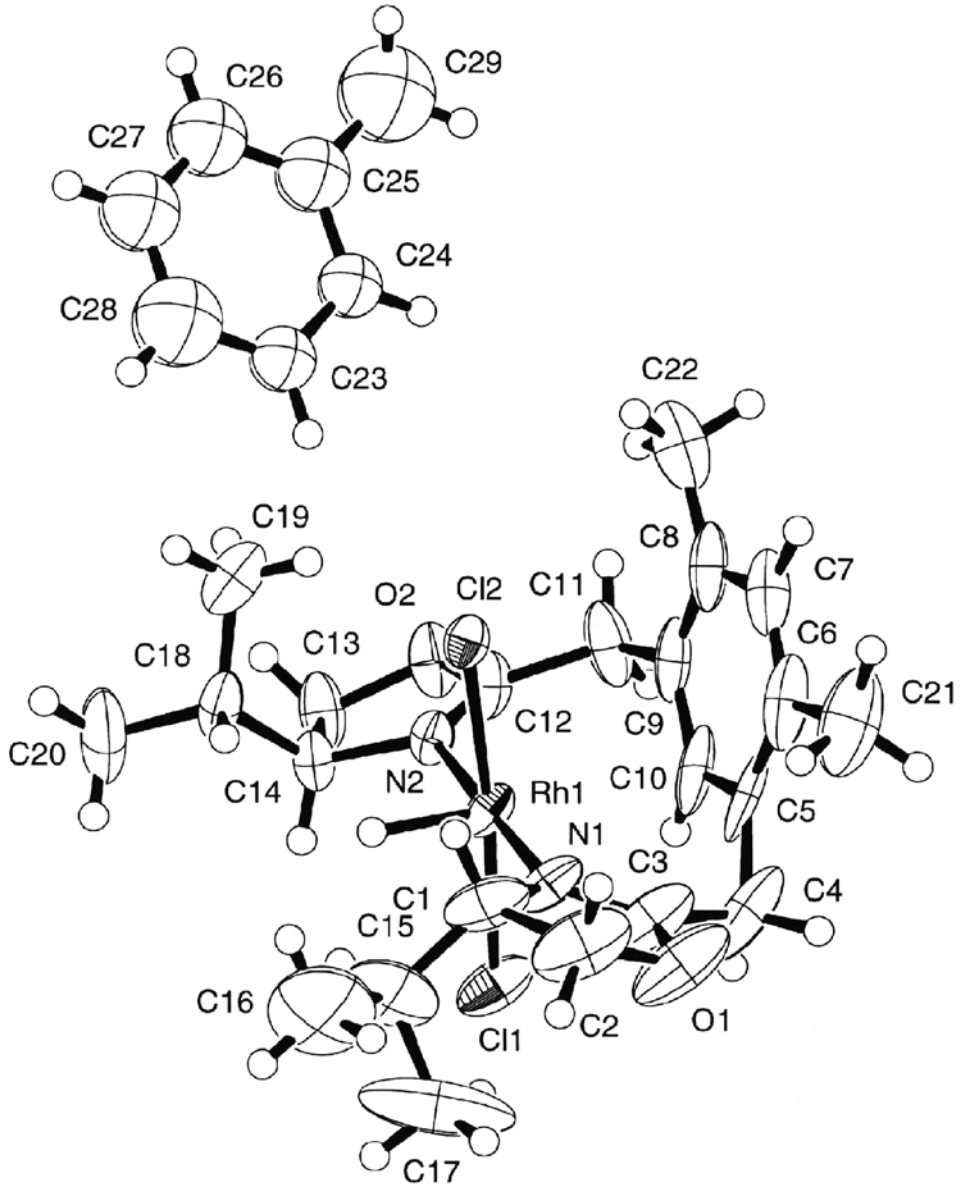

Figure 2. ORTEP diagram of **3b** showing atom numbering scheme and toluene molecule. Thermal ellipsoids are shown at 50% probability.

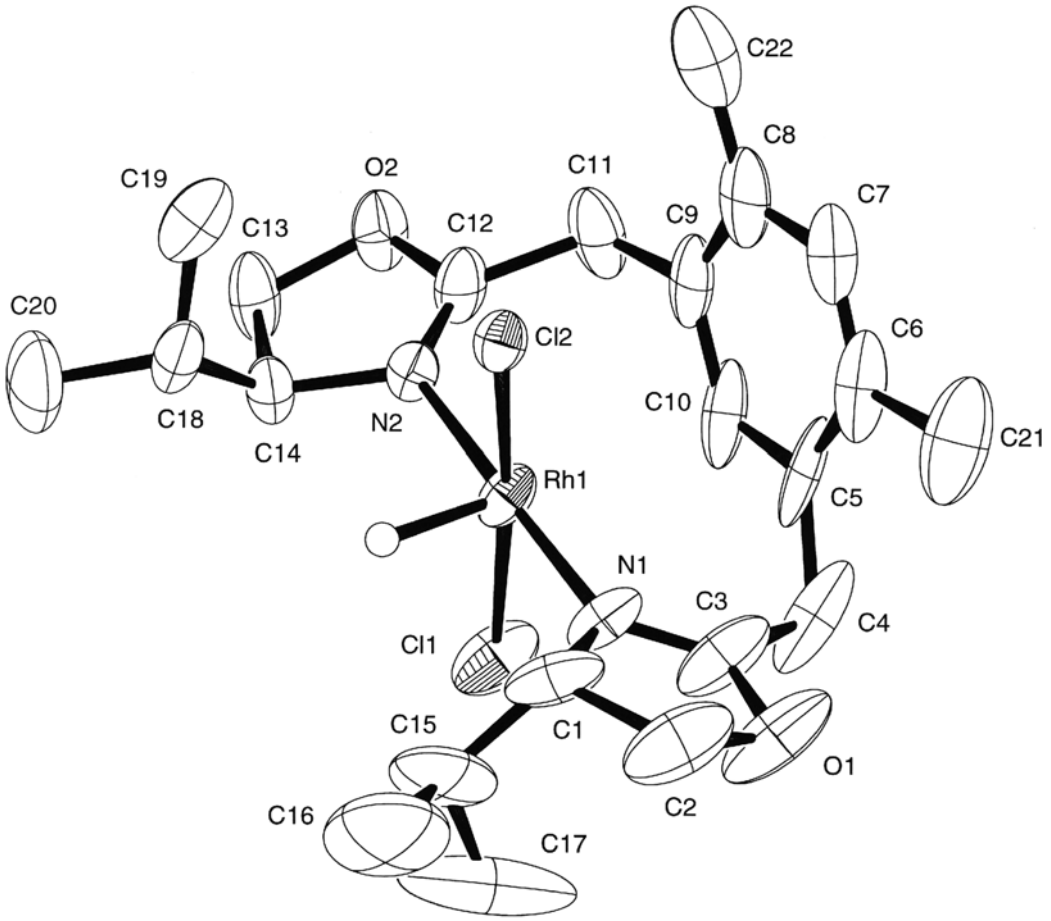

Figure 3. ORTEP diagram of **3b** showing atom numbering scheme. Hydrogen atoms have been omitted for clarity. Thermal ellipsoids are shown at 50% probability.

Table 5: Atomic Coordinates and B*iso*/B*eq* for **3b**.

atom	x	y	z	B(eq)
Rh(1)	0.21129(3)	0.2979	0.22620(3)	2.85(1)
Cl(1)	0.2640(1)	0.1088(3)	0.1604(1)	4.82(6)
Cl(2)	0.16630(9)	0.4789(2)	0.3027(1)	2.74(4)
O(1)	0.3101(3)	0.6501(7)	0.1249(4)	7.2(2)
O(2)	0.0640(2)	-0.0545(5)	0.2174(3)	3.8(1)
N(1)	0.2717(3)	0.4733(9)	0.2039(4)	3.8(2)
N(2)	0.1494(3)	0.1193(7)	0.2446(4)	2.5(1)
C(1)	0.3261(4)	0.5581(10)	0.2693(5)	4.9(2)
C(2)	0.3450(4)	0.691(1)	0.2155(7)	7.0(3)
C(3)	0.2673(5)	0.531(1)	0.1293(6)	5.2(3)
C(4)	0.2179(5)	0.4829(9)	0.0447(5)	6.6(3)
C(5)	0.1503(5)	0.481(1)	0.0593(4)	5.1(2)
C(6)	0.1154(5)	0.6183(9)	0.0680(4)	5.0(2)
C(7)	0.0578(4)	0.6083(9)	0.0941(5)	4.7(2)
C(8)	0.0319(5)	0.467(1)	0.1157(5)	4.9(3)
C(9)	0.0650(4)	0.327(1)	0.1039(4)	4.1(2)
C(10)	0.1212(4)	0.3349(8)	0.0735(4)	4.7(2)
C(11)	0.0422(4)	0.167(1)	0.1242(5)	4.8(2)
C(12)	0.0899(4)	0.0813(8)	0.1986(5)	3.5(2)
C(13)	0.1165(4)	-0.1321(7)	0.2841(5)	4.1(2)
C(14)	0.1755(3)	-0.0104(9)	0.3094(4)	3.2(2)
C(15)	0.3848(4)	0.444(1)	0.3114(7)	6.9(3)
C(16)	0.4403(5)	0.530(2)	0.3824(8)	10.5(4)
C(17)	0.4145(4)	0.367(1)	0.245(1)	13.1(5)
C(18)	0.1915(3)	0.0466(8)	0.4029(4)	3.7(2)
C(19)	0.1334(4)	0.1256(10)	0.4244(4)	5.3(2)
C(20)	0.2193(4)	-0.091(1)	0.4641(5)	6.8(2)
C(21)	0.1415(4)	0.783(1)	0.0486(4)	7.5(2)
C(22)	-0.0255(4)	0.467(1)	0.1540(5)	6.2(2)
C(23)	0.0859(6)	0.529(2)	0.4964(8)	4.9983
C(24)	0.0176(6)	0.520(1)	0.4501(5)	4.7215
C(25)	-0.0313(5)	0.520(1)	0.4944(6)	6.3886
C(26)	-0.0118(6)	0.529(2)	0.5850(6)	6.9983
C(27)	0.0565(7)	0.538(2)	0.6314(5)	7.2498
C(28)	0.1053(5)	0.538(2)	0.5871(8)	9.215
C(29)	-0.1067(5)	0.509(2)	0.443(1)	10.8927
H(1)	0.3087	0.6024	0.3129	5.9204
H(2)	0.3925	0.6941	0.2248	8.364

Table 5: Atomic Coordinates and B*iso*/B*eq* for **3b** (cont.).

atom	x	y	z	B(eq)
H(3)	0.3301	0.7911	0.2302	8.364
H(4)	0.2185	0.5571	0.0005	7.9308
H(5)	0.2288	0.3802	0.0282	7.9308
H(6)	0.0343	0.7038	0.0976	5.6908
H(7)	0.1409	0.2386	0.0619	5.6701
H(8)	0.0006	0.1798	0.1374	5.7071
H(9)	0.0352	0.1025	0.0738	5.7071
H(10)	0.1011	-0.1564	0.3329	4.885
H(11)	0.1303	-0.2271	0.2623	4.885
H(12)	0.2147	-0.056	0.2999	3.788
H(13)	0.3674	0.3612	0.3389	8.2661
H(14)	0.4755	0.4579	0.4085	12.6322
H(15)	0.4578	0.6157	0.357	12.6322
H(16)	0.4214	0.5705	0.4256	12.6322
H(17)	0.3795	0.317	0.2009	15.6827
H(18)	0.4351	0.4467	0.2189	15.6827
H(19)	0.4473	0.2908	0.2727	15.6827
H(20)	0.2266	0.1233	0.4113	4.43
H(21)	0.1479	0.1654	0.4822	6.364
H(22)	0.1172	0.2109	0.3851	6.364
H(23)	0.0981	0.0506	0.4195	6.364
H(24)	0.1867	-0.1736	0.4543	8.177
H(25)	0.2594	-0.1299	0.4536	8.177
H(26)	0.2293	-0.0556	0.5226	8.177
H(27)	0.1856	0.8008	0.0865	9.0412
H(28)	0.1428	0.7863	-0.0101	9.0412
H(29)	0.112	0.864	0.0573	9.0412
H(30)	-0.0133	0.5264	0.2065	7.4618
H(31)	-0.0638	0.5139	0.114	7.4618
H(32)	-0.0357	0.3609	0.1658	7.4618
H(33)	0.0044	0.514	0.3884	5.6811
H(34)	0.1193	0.5297	0.4664	6.0117
H(35)	0.1519	0.5446	0.6187	10.998
H(36)	0.0697	0.5439	0.6931	8.7048
H(37)	-0.0451	0.5282	0.6152	8.3243
H(38)	0.260(2)	0.271(6)	0.312(3)	3.2
H(39)	-0.1122	0.5344	0.3838	13.0215
H(40)	-0.1315	0.5826	0.4668	13.0215
H(41)	-0.1226	0.4047	0.4474	13.0215

Table 6: Anisotropic Displacement Parameters for **3b**.

atom	U11	U22	U33	U12	U13	U23
Rh(1)	0.0488(3)	0.0362(3)	0.0269(2)	-0.0128(4)	0.0165(2)	-0.0073(4)
Cl(1)	0.086(2)	0.055(2)	0.058(2)	-0.016(1)	0.047(1)	-0.023(1)
Cl(2)	0.041(1)	0.034(1)	0.027(1)	-0.0037(10)	0.0081(9)	-0.0022(10)
O(1)	0.136(5)	0.079(4)	0.088(4)	-0.064(4)	0.080(4)	-0.036(4)
O(2)	0.052(3)	0.034(3)	0.046(3)	-0.017(3)	-0.004(3)	0.009(2)
N(1)	0.059(5)	0.051(4)	0.044(4)	-0.022(4)	0.033(4)	-0.011(4)
N(2)	0.033(4)	0.034(4)	0.025(3)	-0.011(3)	0.002(3)	-0.003(3)
C(1)	0.049(5)	0.075(6)	0.077(6)	-0.034(5)	0.039(5)	-0.032(5)
C(2)	0.104(7)	0.069(6)	0.117(8)	-0.046(6)	0.072(7)	-0.024(6)
C(3)	0.096(7)	0.053(6)	0.066(7)	-0.048(5)	0.053(6)	-0.026(5)
C(4)	0.169(9)	0.052(5)	0.049(5)	-0.044(6)	0.063(6)	-0.011(5)
C(5)	0.129(8)	0.051(6)	0.011(4)	-0.039(6)	0.016(4)	0.000(4)
C(6)	0.117(8)	0.030(5)	0.026(4)	-0.025(5)	-0.005(5)	-0.001(4)
C(7)	0.092(7)	0.039(5)	0.034(5)	-0.005(5)	-0.006(5)	0.008(4)
C(8)	0.083(8)	0.063(7)	0.018(5)	-0.015(6)	-0.019(5)	0.003(5)
C(9)	0.072(5)	0.047(7)	0.019(4)	-0.022(5)	-0.013(4)	0.007(4)
C(10)	0.118(6)	0.038(7)	0.012(3)	-0.013(5)	0.001(4)	-0.001(3)
C(11)	0.054(6)	0.051(6)	0.053(6)	-0.014(5)	-0.021(5)	0.014(5)
C(12)	0.057(6)	0.032(5)	0.041(5)	-0.012(4)	0.008(5)	0.010(4)
C(13)	0.068(5)	0.027(4)	0.044(4)	-0.008(4)	-0.007(4)	0.011(3)
C(14)	0.043(4)	0.040(5)	0.031(4)	0.000(4)	0.002(3)	0.009(4)
C(15)	0.028(5)	0.094(8)	0.137(9)	-0.021(5)	0.022(6)	-0.005(7)
C(16)	0.061(7)	0.19(1)	0.15(1)	-0.045(7)	0.029(8)	-0.012(9)
C(17)	0.061(6)	0.13(1)	0.33(2)	-0.020(6)	0.096(9)	-0.09(1)
C(18)	0.048(5)	0.058(5)	0.029(4)	-0.021(4)	0.003(4)	0.011(4)
C(19)	0.090(6)	0.073(6)	0.047(5)	-0.014(5)	0.034(5)	0.000(4)
C(20)	0.081(6)	0.108(7)	0.049(5)	-0.014(5)	-0.014(5)	0.034(5)
C(21)	0.169(8)	0.055(5)	0.055(4)	-0.036(8)	0.022(5)	0.003(6)
C(22)	0.081(6)	0.066(6)	0.067(6)	0.003(5)	-0.015(5)	0.011(5)

Table 7: Bond lengths (Å) for **3b**.

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
Rh(1)	Cl(1)	2.348(3)	1	C(11)	C(12)	1.50(1)	1
Rh(1)	Cl(2)	2.316(2)	1	C(13)	C(14)	1.56(1)	1
Rh(1)	N(1)	2.033(7)	1	C(14)	C(18)	1.517(9)	1
Rh(1)	N(2)	2.052(6)	1	C(15)	C(16)	1.55(1)	1
O(1)	C(2)	1.47(1)	1	C(15)	C(17)	1.52(2)	1
O(1)	C(3)	1.35(1)	1	C(18)	C(19)	1.50(1)	1
O(2)	C(12)	1.334(9)	1	C(18)	C(20)	1.52(1)	1
O(2)	C(13)	1.441(7)	1	C(25)	C(25)	1.25(2)	55602
N(1)	C(1)	1.48(1)	1	C(25)	C(24)	1.40(2)	1
N(1)	C(3)	1.27(1)	1	C(25)	C(24)	0.85(1)	55602
N(2)	C(12)	1.278(9)	1	C(25)	C(23)	1.18(2)	55602
N(2)	C(14)	1.497(9)	1	C(25)	C(28)	1.71(1)	55602
C(1)	C(2)	1.53(1)	1	C(25)	C(26)	1.40(1)	1
C(1)	C(15)	1.54(1)	1	C(25)	C(26)	1.76(2)	55602
C(3)	C(4)	1.50(1)	1	C(25)	C(29)	1.54(1)	1
C(4)	C(5)	1.48(2)	1	C(24)	C(23)	1.40(2)	1
C(5)	C(6)	1.39(1)	1	C(24)	C(27)	1.71(1)	55602
C(5)	C(10)	1.42(1)	1	C(24)	C(26)	0.55(1)	55602
C(6)	C(7)	1.38(1)	1	C(23)	C(28)	1.40(2)	1
C(6)	C(21)	1.56(1)	1	C(23)	C(26)	1.70(1)	55602
C(7)	C(8)	1.39(1)	1	C(23)	C(29)	0.95(2)	55602
C(8)	C(9)	1.40(1)	1	C(28)	C(27)	1.40(2)	1
C(8)	C(22)	1.49(1)	1	C(28)	C(29)	0.55(2)	55602
C(9)	C(10)	1.39(1)	1	C(27)	C(26)	1.40(2)	1
C(9)	C(11)	1.50(1)	1	C(27)	C(29)	1.81(2)	55602

Table 7: Bond lengths (Å) for **3b** (cont.).

atom	atom	distance	atom	atom	distance
Rh1	H38	1.47	C17	H17	0.949
C1	H1	0.95	C17	H18	0.949
C2	H2	0.95	C17	H19	0.951
C2	H3	0.95	C18	H20	0.95
C4	H4	0.95	C19	H21	0.95
C4	H5	0.95	C19	H22	0.95
C7	H6	0.95	C19	H23	0.951
C10	H7	0.95	C20	H24	0.95
C11	H8	0.951	C20	H25	0.951
C11	H9	0.949	C20	H26	0.95
C13	H10	0.95	C21	H27	0.949
C13	H11	0.95	C21	H28	0.95
C14	H12	0.95	C21	H29	0.95
C15	H13	0.949	C22	H30	0.949
C16	H14	0.949	C22	H31	0.948
C16	H15	0.949	C22	H32	0.951
C16	H16	0.952			

Table 8: Bond angles (°) for **3b**.

atom	atom	atom	angle	atom	atom	atom	angle
Cl1	Rh1	Cl2	174.93(7)	C5	C6	C21	120.2(9)
Cl1	Rh1	N1	91.3(2)	C7	C6	C21	119.8(8)
Cl1	Rh1	N2	87.6(2)	C6	C7	C8	123.9(8)
Cl2	Rh1	N1	88.8(2)	C7	C8	C9	116.5(9)
Cl2	Rh1	N2	92.4(2)	C7	C8	C22	120.8(9)
N1	Rh1	N2	178.2(2)	C9	C8	C22	122.6(9)
C2	O1	C3	105.3(7)	C8	C9	C10	120.1(8)
C12	O2	C13	107.0(5)	C8	C9	C11	122.1(8)
Rh1	N1	C1	127.2(5)	C10	C9	C11	117.8(8)
Rh1	N1	C3	124.5(6)	C5	C10	C9	122.4(8)
C1	N1	C3	108.4(7)	C9	C11	C12	115.6(6)
Rh1	N2	C12	129.6(5)	O2	C12	N2	117.8(6)
Rh1	N2	C14	121.4(4)	O2	C12	C11	112.2(6)
C12	N2	C14	108.1(6)	N2	C12	C11	130.0(7)
N1	C1	C2	102.6(6)	O2	C13	C14	105.1(5)
N1	C1	C15	110.4(7)	N2	C14	C13	101.6(5)
C2	C1	C15	113.8(8)	N2	C14	C18	112.8(6)
O1	C2	C1	104.7(6)	C13	C14	C18	113.4(6)
O1	C3	N1	117.7(7)	C1	C15	C16	110.5(8)
O1	C3	C4	116.0(8)	C1	C15	C17	112.5(8)
N1	C3	C4	126.3(9)	C16	C15	C17	110.8(8)
C3	C4	C5	106.6(8)	C14	C18	C19	114.1(5)
C4	C5	C6	123.1(8)	C14	C18	C20	109.4(6)
C4	C5	C10	120.0(8)	C19	C18	C20	111.5(7)
C6	C5	C10	116.6(9)	C5	C6	C7	120.0(8)
Cl1	Rh1	H38	91.65	N1	Rh1	H38	89.11
Cl2	Rh1	H38	83.28	N2	Rh1	H38	92.43

Table 8: Bond angles (^{o}) for **3b** (cont.).

atom	atom	atom	angle	atom	atom	atom	angle
O2	C13	H10	110.51	C14	C13	H10	110.61
O2	C13	H11	110.52	C14	C13	H11	110.62
N1	C1	H1	109.93	H10	C13	H11	109.46
C2	C1	H1	109.93	N2	C14	H12	109.58
C15	C1	H1	109.9	C13	C14	H12	109.57
O1	C2	H2	110.62	C18	C14	H12	109.56
O1	C2	H3	110.66	C1	C15	H13	107.6
C1	C2	H2	110.63	C16	C15	H13	107.6
C1	C2	H3	110.68	C17	C15	H13	107.69
H2	C2	H3	109.47	C15	C16	H14	109.52
C3	C4	H4	110.18	C15	C16	H15	109.56
C3	C4	H5	110.18	C15	C16	H16	109.41
C5	C4	H4	110.16	H14	C16	H15	109.58
C5	C4	H5	110.16	H14	C16	H16	109.38
H4	C4	H5	109.5	H15	C16	H16	109.38
C6	C7	H6	118.06	C15	C17	H17	109.41
C8	C7	H6	118	C15	C17	H18	109.49
C5	C10	H7	118.84	C15	C17	H19	109.34
C9	C10	H7	118.77	H17	C17	H18	109.61
C9	C11	H8	107.89	H17	C17	H19	109.46
C9	C11	H9	107.99	H18	C17	H19	109.51
C12	C11	H8	107.86	C14	C18	H20	107.2
C12	C11	H9	107.98	C19	C18	H20	107.14
H8	C11	H9	109.41	C20	C18	H20	107.23
C18	C19	H21	109.53	H25	C20	H26	109.44
C18	C19	H22	109.54	C6	C21	H27	109.47
C18	C19	H23	109.5	C6	C21	H28	109.41
H21	C19	H22	109.44	C6	C21	H29	109.45
H21	C19	H23	109.41	H27	C21	H28	109.5
H22	C19	H23	109.41	H27	C21	H29	109.54
C18	C20	H24	109.5	H28	C21	H29	109.46
C18	C20	H25	109.41	C8	C22	H30	109.38
C18	C20	H26	109.51	C8	C22	H31	109.43
H24	C20	H25	109.43	C8	C22	H32	109.28
H24	C20	H26	109.54	H30	C22	H31	109.68
H30	C22	H32	109.5	H31	C22	H32	109.56

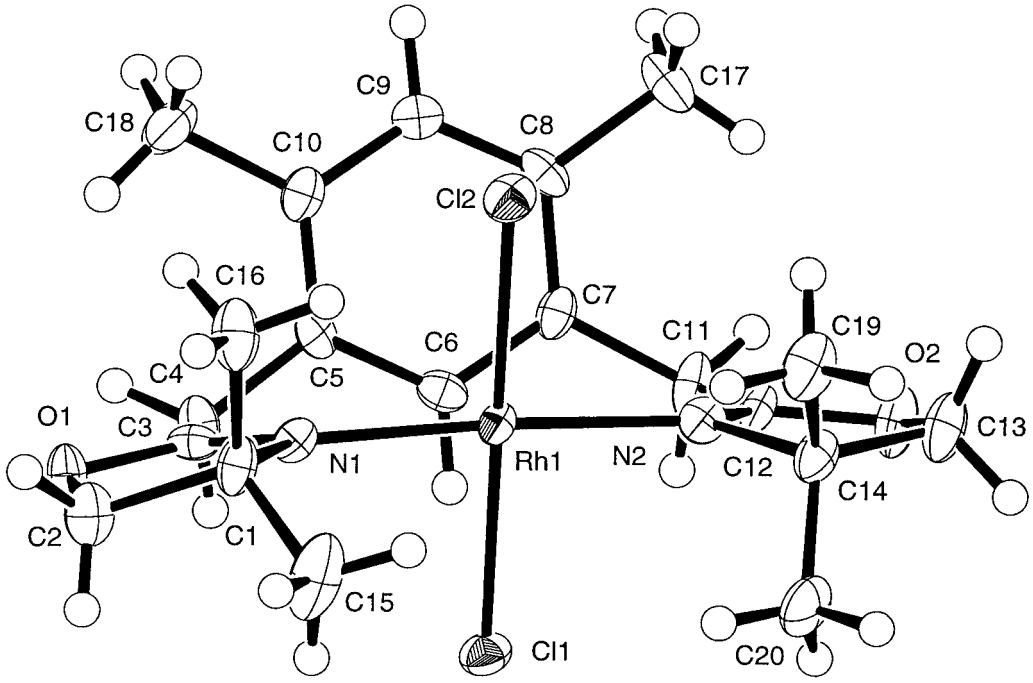

Figure 4. ORTEP diagram of **3c** showing atom numbering scheme. Thermal ellipsoids are shown at 50% probability.

Table 9: Atomic Coordinates and B*iso*/B*eq* for **3c**.

atom	x	y	z	B(eq)
Rh(1)	0.77287(5)	0.4002	0.74000(5)	1.263(9)
Cl(1)	0.9347(2)	0.2684(1)	0.6668(2)	1.94(4)
Cl(2)	0.6127(2)	0.5362(1)	0.8025(2)	1.97(4)
O(1)	1.1773(5)	0.5389(4)	0.9029(5)	1.8(1)
O(2)	0.4308(5)	0.1646(4)	0.6790(5)	2.5(1)
N(1)	0.9577(6)	0.4931(5)	0.7884(6)	1.4(1)
N(2)	0.5937(6)	0.3028(4)	0.6801(6)	1.6(1)
C(1)	1.0197(8)	0.5782(5)	0.7030(8)	1.8(2)
C(2)	1.1799(8)	0.5906(6)	0.7697(8)	2.3(2)
C(3)	1.0503(7)	0.4799(5)	0.8969(7)	1.5(2)
C(4)	1.0390(6)	0.404(1)	1.0104(6)	1.8(1)
C(5)	0.8798(6)	0.3802(6)	1.0338(7)	1.5(2)
C(6)	0.8088(7)	0.2919(5)	0.9675(7)	1.6(2)
C(7)	0.6594(7)	0.2735(5)	0.9727(7)	1.6(2)
C(8)	0.5785(7)	0.3399(6)	1.0527(7)	1.6(2)
C(9)	0.6520(7)	0.4238(5)	1.1236(7)	1.6(2)
C(10)	0.8009(7)	0.4482(5)	1.1124(7)	1.7(2)
C(11)	0.5887(8)	0.1843(6)	0.8823(7)	2.1(2)
C(12)	0.5424(8)	0.2228(5)	0.7443(7)	1.6(2)
C(13)	0.3877(9)	0.2238(6)	0.5520(8)	2.6(2)
C(14)	0.5146(8)	0.3017(6)	0.5368(7)	1.9(2)
C(15)	1.0207(10)	0.5410(7)	0.5560(8)	3.5(2)
C(16)	0.9330(8)	0.6835(6)	0.7135(8)	2.8(2)
C(17)	0.4131(7)	0.3263(6)	1.0561(9)	2.7(2)
C(18)	0.8712(9)	0.5483(7)	1.1805(9)	3.0(2)
C(19)	0.4583(8)	0.4156(9)	0.4952(8)	2.6(2)
C(20)	0.6198(8)	0.2573(7)	0.4387(8)	2.8(2)

Table 9: Atomic Coordinates and B*iso*/B*eq* for **3c** (cont.).

atom	x	y	z	B(eq)
H(1)	1.2062	0.6653	0.7791	2.7956
H(2)	1.2479	0.5545	0.7174	2.7956
H(3)	1.0863	0.3374	0.9907	2.2103
H(4)	1.0874	0.4349	1.0906	2.2103
H(5)	0.8645	0.2432	0.9175	1.9638
H(6)	0.599	0.4668	1.1825	1.9484
H(7)	0.6582	0.127	0.877	2.5003
H(8)	0.5041	0.1577	0.9216	2.5003
H(9)	0.3759	0.1749	0.4774	3.1252
H(10)	0.298	0.2627	0.5583	3.1252
H(11)	0.9223	0.5259	0.5195	4.2499
H(12)	1.0612	0.597	0.5044	4.2499
H(13)	1.0792	0.4771	0.5527	4.2499
H(14)	0.9399	0.7068	0.8054	3.3484
H(15)	0.9728	0.738	0.6593	3.3484
H(16)	0.8321	0.6713	0.6823	3.3484
H(17)	0.364	0.3899	1.0204	3.2608
H(18)	0.3805	0.265	1.0029	3.2608
H(19)	0.3911	0.3155	1.1471	3.2608
H(20)	0.9723	0.552	1.1633	3.6455
H(21)	0.821	0.6116	1.1453	3.6455
H(22)	0.8643	0.5441	1.2755	3.6455
H(23)	0.5403	0.4626	0.4869	3.1565
H(24)	0.3998	0.4115	0.4106	3.1565
H(25)	0.4	0.4434	0.5623	3.1565
H(26)	0.6491	0.1854	0.4649	3.327
H(27)	0.5712	0.256	0.3494	3.327
H(28)	0.7048	0.3026	0.4405	3.327

Table 10: Anisotropic Displacement Parameters for **3c**.

atom	U11	U22	U33	U12	U13	U23
Rh(1)	0.0190(2)	0.0125(2)	0.0155(3)	0.0013(3)	-0.0036(2)	0.0000(3)
Cl(1)	0.028(1)	0.0198(9)	0.026(1)	0.0056(8)	0.0013(9)	-0.0033(9)
Cl(2)	0.029(1)	0.0187(9)	0.026(1)	0.0069(8)	-0.0030(9)	0.0007(9)
O(1)	0.021(3)	0.025(3)	0.023(3)	-0.009(2)	-0.002(2)	0.005(2)
O(2)	0.038(3)	0.029(3)	0.025(3)	-0.012(2)	-0.012(2)	0.004(2)
N(1)	0.024(3)	0.017(3)	0.011(3)	0.000(2)	0.000(3)	0.002(3)
N(2)	0.023(3)	0.017(3)	0.020(4)	0.005(2)	-0.003(3)	0.004(3)
C(1)	0.029(4)	0.019(4)	0.020(4)	-0.008(3)	-0.005(3)	0.004(3)
C(2)	0.031(4)	0.032(4)	0.025(5)	-0.006(3)	-0.003(4)	0.006(4)
C(3)	0.021(4)	0.019(4)	0.019(4)	0.003(3)	0.009(3)	0.001(3)
C(4)	0.020(3)	0.025(4)	0.024(4)	-0.004(5)	-0.004(3)	0.007(5)
C(5)	0.016(3)	0.025(5)	0.015(3)	0.004(3)	-0.006(3)	0.007(3)
C(6)	0.020(4)	0.020(4)	0.023(4)	0.006(3)	0.003(3)	0.004(3)
C(7)	0.026(4)	0.014(3)	0.021(4)	-0.005(3)	-0.003(3)	0.001(3)
C(8)	0.014(4)	0.023(4)	0.024(4)	0.006(3)	0.000(3)	0.011(3)
C(9)	0.025(4)	0.019(5)	0.018(4)	0.002(3)	0.003(3)	0.004(3)
C(10)	0.027(4)	0.022(3)	0.014(4)	-0.003(3)	-0.005(3)	0.003(3)
C(11)	0.034(4)	0.017(4)	0.025(5)	-0.008(3)	-0.013(3)	0.005(3)
C(12)	0.024(4)	0.016(4)	0.018(4)	-0.003(3)	-0.005(3)	-0.004(3)
C(13)	0.039(5)	0.032(5)	0.025(5)	-0.007(3)	-0.015(4)	0.000(4)
C(14)	0.029(4)	0.022(4)	0.020(4)	0.002(3)	-0.008(3)	-0.001(3)
C(15)	0.066(6)	0.046(5)	0.021(5)	-0.026(5)	-0.006(4)	0.009(4)
C(16)	0.034(4)	0.035(5)	0.035(5)	-0.007(3)	-0.013(4)	0.007(4)
C(17)	0.016(4)	0.040(5)	0.047(6)	-0.001(3)	0.003(4)	0.006(4)
C(18)	0.044(5)	0.036(5)	0.036(5)	-0.010(4)	0.008(4)	-0.019(4)
C(19)	0.044(4)	0.027(6)	0.025(4)	0.000(4)	-0.014(3)	0.006(4)
C(20)	0.040(5)	0.042(5)	0.020(5)	0.002(4)	-0.011(4)	-0.008(4)

Table 11: Bond lengths (Å) for **3c**.

atom	atom	distance	atom	atom	distance
Rh1	Cl1	2.344(2)	C3	C4	1.47(1)
Rh1	Cl2	2.334(2)	C4	C5	1.513(8)
Rh1	N1	2.048(6)	C5	C6	1.39(1)
Rh1	N2	2.060(6)	C5	C10	1.385(9)
O1	C2	1.465(9)	C6	C7	1.380(9)
O1	C3	1.357(8)	C7	C8	1.39(1)
O2	C12	1.353(8)	C7	C11	1.517(9)
O2	C13	1.473(9)	C8	C9	1.382(9)
N1	C1	1.487(8)	C8	C17	1.513(9)
N1	C3	1.310(9)	C9	C10	1.398(9)
N2	C12	1.280(8)	C10	C18	1.51(1)
N2	C14	1.529(9)	C11	C12	1.47(1)
C1	C2	1.55(1)	C13	C14	1.51(1)
C1	C15	1.52(1)	C14	C19	1.53(1)
C1	C16	1.52(1)	C14	C20	1.53(1)
C2	H1	0.95	C16	H15	0.95
C2	H2	0.95	C16	H16	0.95
C4	H3	0.95	C17	H17	0.95
C4	H4	0.95	C17	H18	0.95
C6	H5	0.95	C17	H19	0.95
C9	H6	0.95	C18	H20	0.95
C11	H7	0.95	C18	H21	0.95
C11	H8	0.95	C18	H22	0.95
C13	H9	0.95	C19	H23	0.95
C13	H10	0.95	C19	H24	0.95
C15	H11	0.95	C19	H25	0.95
C15	H12	0.95	C20	H26	0.95
C15	H13	0.95	C20	H27	0.95
C16	H14	0.95	C20	H28	0.95

Table 12: Bond angles (°) for **3c**.

atom	atom	atom	angle	atom	atom	atom	angle
Cl1	Rh1	Cl2	177.06(7)	C4	C5	C6	118.9(7)
Cl1	Rh1	N1	86.2(2)	C4	C5	C10	121.4(7)
Cl1	Rh1	N2	90.6(2)	C6	C5	C10	119.5(6)
Cl2	Rh1	N1	93.2(2)	C5	C6	C7	121.5(6)
Cl2	Rh1	N2	89.8(2)	C6	C7	C8	119.8(6)
N1	Rh1	N2	176.1(2)	C6	C7	C11	117.3(6)
C2	O1	C3	106.0(5)	C8	C7	C11	122.8(6)
C12	O2	C13	105.9(5)	C7	C8	C9	118.0(6)
Rh1	N1	C1	127.1(4)	C7	C8	C17	121.7(7)
Rh1	N1	C3	124.8(4)	C9	C8	C17	120.3(7)
C1	N1	C3	107.8(5)	C8	C9	C10	123.0(6)
Rh1	N2	C12	128.0(5)	C5	C10	C9	118.0(6)
Rh1	N2	C14	124.2(4)	C5	C10	C18	121.4(6)
C12	N2	C14	107.0(6)	C9	C10	C18	120.6(6)
N1	C1	C2	102.5(6)	C7	C11	C12	112.7(6)
N1	C1	C15	111.6(6)	O2	C12	N2	117.3(6)
N1	C1	C16	109.4(6)	O2	C12	C11	114.3(6)
C2	C1	C15	110.3(6)	N2	C12	C11	128.5(7)
C2	C1	C16	111.1(6)	O2	C13	C14	104.6(6)
C15	C1	C16	111.6(7)	N2	C14	C13	102.1(6)
O1	C2	C1	104.4(5)	N2	C14	C19	110.9(6)
O1	C3	N1	116.5(6)	N2	C14	C20	109.0(5)
O1	C3	C4	115.1(6)	C13	C14	C19	111.5(6)
N1	C3	C4	128.3(6)	C13	C14	C20	111.4(6)
C3	C4	C5	112.0(6)	C19	C14	C20	111.6(6)
O1	C2	H1	110.73	C1	C15	H13	109.48
O1	C2	H2	110.74	H11	C15	H12	109.46

Table 12: Bond angles (°) for **3c** (cont.).

atom	atom	atom	angle	atom	atom	atom	angle
C1	C2	H1	110.73	H11	C15	H13	109.5
C1	C2	H2	110.73	H12	C15	H13	109.48
H1	C2	H2	109.47	C1	C16	H14	109.46
C3	C4	H3	108.86	C1	C16	H15	109.46
C3	C4	H4	108.85	C1	C16	H16	109.46
C5	C4	H3	108.85	H14	C16	H15	109.49
C5	C4	H4	108.83	H14	C16	H16	109.49
H3	C4	H4	109.46	H15	C16	H16	109.48
C5	C6	H5	119.29	C8	C17	H17	109.48
C7	C6	H5	119.26	C8	C17	H18	109.47
C8	C9	H6	118.52	C8	C17	H19	109.47
C10	C9	H6	118.52	H17	C17	H18	109.47
C7	C11	H7	108.67	H17	C17	H19	109.47
C7	C11	H8	108.65	H18	C17	H19	109.46
C12	C11	H7	108.69	C10	C18	H20	109.45
C12	C11	H8	108.67	C10	C18	H21	109.47
H7	C11	H8	109.47	C10	C18	H22	109.45
O2	C13	H9	110.67	H20	C18	H21	109.48
O2	C13	H10	110.65	H20	C18	H22	109.48
C14	C13	H9	110.68	H21	C18	H22	109.49
C14	C13	H10	110.68	C14	C19	H23	109.45
H9	C13	H10	109.47	C14	C19	H24	109.45
C1	C15	H11	109.46	C14	C19	H25	109.46
C1	C15	H12	109.45	H23	C19	H24	109.49
H23	C19	H25	109.49	C14	C20	H28	109.46
H24	C19	H25	109.49	H26	C20	H27	109.48
C14	C20	H26	109.48	H26	C20	H28	109.46
C14	C20	H27	109.48	H27	C20	H28	109.46