

Experimental Details for X-ray crystallography of 4·CH₂Cl₂.

Singles crystals of **4** (CH₂Cl₂-hexane) were obtained by recrystallization from the solvent systems shown in the parentheses and mounted on glass fibers. The crystallographic data are summarized in Table S1.

Diffraction measurement of **4** was made on a Rigaku RAXIS IV imaging plate area detector with Mo K α radiation (λ = 0.71069 Å). All the data collections were carried out at -60°C. Indexing was performed from 3 oscillation images which were exposed for 4 min. The crystal-to-detector distance was 110 mm. Data collection parameters were as follows: the oscillation range: 3.5°; the number of oscillation images: 31; the exposed time: 45 min. Readout was performed with the pixel size of 100 μ m x 100 μ m. Neutral scattering factors were obtained from the standard source.¹ In the reduction of data, Lorentz, polarization, and empirical absorption corrections were made.²

The structures were solved by a combination of the direct methods (SHELXL 86) and Fourier synthesis (DIRDIF). Least-squares refinements were carried out using SHELEXL93 linked to teXsan. All the non-hydrogen atoms were refined anisotropically. The methyl hydrogen atoms were refined using the riding models and the other hydrogen atoms were fixed at the calculated positions and not refined.

- (1) International Tables for X-Ray Crystallography; Kynoch Press: Birmingham, 1975; Vol. 4.
- (2) Stuart, D.; Walker, N. *Acta Cryst.* **1979**, A35, 925.

Table S1. Crystallographic data for 4·CH₂Cl₂.

formula	C ₅₄ H ₇₀ BN ₆ P ₂ Cl ₂ Rh	d _{calcd} / g·cm ⁻³	1.23
formula weight	1049.72	μ / cm ⁻¹	0.489
crystal system	monoclinic	2θ / deg	up to 55.06
space group	C2/c	no of parameters	607
a / Å	40.548(6)	refined	
b / Å	14.205(4)	R1	0.0723
c / Å	24.967(11)	for data with F _o > 4σ(F _o)	(8382 data)
β / deg	127.675(15)	wR2	0.2003
V / Å ³	11381.9(60)	for all data	(9819 data)
Z	8		

Table S2. Positional parameters and B_{eq} for 4.

ATOM	X	Y	Z	B (EQ)
Rh(1)	0.16430(1)	0.17907(3)	0.25918(2)	1.99(1)
Cl(1)	0.0546(2)	0.4950(3)	0.2621(4)	15.8(2)
Cl(2)	0.1338(3)	0.5222(5)	0.3943(3)	18.9(3)
P(1)	0.21880(4)	0.1552(1)	0.26127(7)	2.26(3)
P(2)	0.15855(4)	0.02364(9)	0.25230(7)	2.16(2)
N(11)	0.1091(1)	0.2091(3)	0.2487(2)	2.12(7)
N(12)	0.0797(1)	0.2642(3)	0.1939(2)	1.89(7)
N(21)	0.1671(1)	0.3270(3)	0.2642(2)	2.34(8)
N(22)	0.1333(1)	0.3782(3)	0.2135(2)	2.02(7)
N(31)	0.1069(1)	0.1946(3)	0.1133(2)	2.13(7)
N(32)	0.0893(1)	0.2817(3)	0.1015(2)	2.00(7)
C(1)	0.2230(2)	0.0319(4)	0.2467(3)	2.8(1)
C(2)	0.1959(2)	-0.0269(4)	0.2426(3)	2.7(1)
C(11)	0.0914(2)	0.1764(4)	0.2759(3)	2.64(10)
C(12)	0.0504(2)	0.2081(4)	0.2386(3)	2.8(1)
C(13)	0.0439(2)	0.2626(4)	0.1875(3)	2.41(9)
C(14)	0.1156(2)	0.1191(5)	0.3396(3)	3.5(1)
C(15)	0.1280(3)	0.1770(6)	0.4002(4)	5.2(2)
C(16)	0.0915(3)	0.0342(6)	0.3337(5)	5.9(2)
C(17)	0.0039(2)	0.3067(5)	0.1292(3)	3.1(1)
C(18)	-0.0262(2)	0.3194(7)	0.1459(5)	5.2(2)
C(19)	-0.0161(3)	0.2506(8)	0.0658(4)	6.2(2)
C(21)	0.1949(2)	0.3878(4)	0.3119(3)	2.29(9)
C(22)	0.1795(2)	0.4798(4)	0.2905(3)	2.8(1)
C(23)	0.1413(2)	0.4713(4)	0.2293(3)	2.33(9)
C(24)	0.2332(2)	0.3580(4)	0.3783(3)	3.2(1)
C(25)	0.2246(3)	0.3390(6)	0.4284(4)	5.4(2)
C(26)	0.2681(2)	0.4292(5)	0.4070(4)	3.8(1)
C(27)	0.1132(2)	0.5506(4)	0.1838(3)	2.7(1)
C(28)	0.1170(3)	0.6353(5)	0.2256(5)	5.8(2)
C(29)	0.1232(3)	0.5786(7)	0.1373(5)	5.4(2)
C(31)	0.1023(2)	0.1721(4)	0.0571(3)	2.37(9)
C(32)	0.0819(2)	0.2435(4)	0.0096(3)	2.9(1)
C(33)	0.0735(2)	0.3123(4)	0.0384(3)	2.45(9)
C(34)	0.1186(2)	0.0811(4)	0.0514(3)	3.0(1)
C(35)	0.1439(2)	0.0966(5)	0.0262(4)	4.0(1)
C(36)	0.0829(2)	0.0126(5)	0.0050(4)	3.8(1)
C(37)	0.0509(2)	0.4040(4)	0.0073(3)	3.1(1)
C(38)	0.0661(4)	0.4510(7)	-0.0287(6)	6.5(2)
C(39)	0.0050(3)	0.3895(6)	-0.0404(6)	6.6(3)
C(41)	0.2207(2)	0.2167(4)	0.1984(3)	2.68(10)
C(42)	0.1942(2)	0.2906(4)	0.1620(3)	3.0(1)
C(43)	0.1958(2)	0.3385(5)	0.1151(4)	3.7(1)
C(44)	0.2247(3)	0.3103(5)	0.1049(4)	4.2(1)
C(45)	0.2513(2)	0.2363(5)	0.1420(4)	3.9(1)
C(46)	0.2494(2)	0.1901(5)	0.1881(4)	3.4(1)
C(51)	0.2726(2)	0.1730(5)	0.3376(3)	3.0(1)
C(52)	0.2949(2)	0.2549(5)	0.3458(4)	3.7(1)
C(53)	0.3351(3)	0.2687(7)	0.4065(5)	5.6(2)
C(54)	0.3530(3)	0.2075(9)	0.4576(4)	5.9(2)
C(55)	0.3304(3)	0.1242(8)	0.4494(4)	6.1(2)
C(56)	0.2907(2)	0.1088(6)	0.3899(4)	4.2(1)

Table S2. Positional parameters and B_{eq} for 4. (cont'd.)

ATOM	X	Y	Z	B (EQ)
C (61)	0.1093 (2)	-0.0299 (4)	0.1822 (3)	2.53 (10)
C (62)	0.0724 (2)	0.0205 (4)	0.1526 (3)	3.0 (1)
C (63)	0.0346 (2)	-0.0188 (5)	0.1017 (4)	3.7 (1)
C (64)	0.0318 (2)	-0.1078 (5)	0.0773 (4)	4.1 (1)
C (65)	0.0686 (3)	-0.1577 (4)	0.1054 (4)	3.8 (1)
C (66)	0.1071 (2)	-0.1189 (4)	0.1575 (3)	3.2 (1)
C (71)	0.1735 (2)	-0.0455 (4)	0.3270 (3)	2.7 (1)
C (72)	0.1542 (3)	-0.1299 (5)	0.3217 (4)	3.7 (1)
C (73)	0.1680 (3)	-0.1790 (5)	0.3805 (5)	4.9 (2)
C (74)	0.1997 (3)	-0.1461 (6)	0.4423 (4)	5.1 (2)
C (75)	0.2190 (3)	-0.0601 (6)	0.4473 (4)	4.4 (2)
C (76)	0.2052 (2)	-0.0118 (5)	0.3895 (3)	3.2 (1)
C (81)	0.1027 (7)	0.4434 (9)	0.327 (1)	11.5 (6)
B (1)	0.0904 (2)	0.3307 (4)	0.1574 (3)	2.15 (10)

Table S3. Anisotropic thermal parameters for 4.

ATOM	U11	U22	U33	U12	U13	U23
Rh(1)	0.0224(2)	0.0231(2)	0.0279(2)	0.0015(2)	0.0141(2)	0.0003(2)
Cl(1)	0.182(5)	0.105(3)	0.367(9)	-0.020(3)	0.194(7)	-0.003(4)
Cl(2)	0.40(1)	0.234(6)	0.181(5)	0.158(7)	0.223(7)	0.100(5)
P(1)	0.0220(7)	0.0300(7)	0.0318(7)	0.0018(5)	0.0154(6)	0.0009(6)
P(2)	0.0269(8)	0.0249(6)	0.0291(7)	0.0013(5)	0.0164(6)	0.0010(6)
N(11)	0.027(2)	0.027(2)	0.030(2)	0.003(2)	0.019(2)	0.002(2)
N(12)	0.018(2)	0.029(2)	0.023(2)	0.002(2)	0.012(2)	0.004(2)
N(21)	0.023(2)	0.028(2)	0.028(2)	0.001(2)	0.011(2)	-0.001(2)
N(22)	0.022(2)	0.025(2)	0.028(2)	0.002(2)	0.015(2)	0.003(2)
N(31)	0.024(2)	0.027(2)	0.026(2)	0.004(2)	0.013(2)	0.002(2)
N(32)	0.023(2)	0.025(2)	0.027(2)	0.002(2)	0.015(2)	0.004(2)
C(1)	0.041(4)	0.034(3)	0.040(3)	0.007(2)	0.028(3)	0.004(3)
C(2)	0.037(3)	0.031(3)	0.039(3)	0.006(2)	0.025(3)	0.003(2)
C(11)	0.040(3)	0.034(3)	0.032(3)	0.011(2)	0.025(3)	0.010(2)
C(12)	0.033(3)	0.045(3)	0.041(3)	0.008(2)	0.029(3)	0.012(3)
C(13)	0.021(3)	0.040(3)	0.032(3)	0.001(2)	0.017(2)	0.004(2)
C(14)	0.054(4)	0.052(4)	0.042(4)	0.023(3)	0.037(4)	0.017(3)
C(15)	0.067(6)	0.093(6)	0.036(4)	0.028(5)	0.032(4)	0.019(4)
C(16)	0.100(8)	0.060(5)	0.075(6)	0.006(5)	0.060(6)	0.027(5)
C(17)	0.025(3)	0.055(4)	0.041(3)	0.004(3)	0.022(3)	0.013(3)
C(18)	0.038(4)	0.097(6)	0.073(5)	0.027(4)	0.040(4)	0.039(5)
C(19)	0.037(5)	0.126(8)	0.044(4)	0.010(5)	0.011(4)	-0.007(5)
C(21)	0.024(3)	0.028(3)	0.028(3)	0.000(2)	0.013(2)	-0.003(2)
C(22)	0.036(3)	0.028(3)	0.040(3)	-0.005(2)	0.022(3)	-0.003(2)
C(23)	0.027(3)	0.028(3)	0.035(3)	0.000(2)	0.020(3)	0.002(2)
C(24)	0.032(3)	0.033(3)	0.037(3)	0.001(2)	0.011(3)	0.003(3)
C(25)	0.067(6)	0.069(5)	0.042(4)	-0.016(4)	0.020(4)	0.016(4)
C(26)	0.030(4)	0.053(4)	0.039(3)	-0.004(3)	0.011(3)	-0.007(3)
C(27)	0.028(3)	0.027(3)	0.044(3)	0.001(2)	0.019(3)	0.001(2)
C(28)	0.090(7)	0.042(4)	0.076(6)	0.026(4)	0.043(6)	0.011(4)
C(29)	0.056(5)	0.085(6)	0.059(5)	0.018(4)	0.032(5)	0.034(5)
C(31)	0.025(3)	0.031(3)	0.033(3)	0.000(2)	0.017(2)	-0.001(2)
C(32)	0.039(4)	0.042(3)	0.028(3)	0.008(2)	0.019(3)	0.003(2)
C(33)	0.034(3)	0.033(3)	0.029(3)	0.000(2)	0.021(2)	0.003(2)
C(34)	0.037(4)	0.036(3)	0.031(3)	0.009(2)	0.016(3)	0.001(2)
C(35)	0.041(4)	0.060(4)	0.057(4)	0.003(3)	0.033(4)	-0.011(3)
C(36)	0.046(4)	0.040(3)	0.053(4)	-0.002(3)	0.028(4)	-0.006(3)
C(37)	0.041(4)	0.039(3)	0.033(3)	0.009(3)	0.019(3)	0.011(3)
C(38)	0.106(9)	0.068(5)	0.106(8)	0.032(5)	0.081(8)	0.045(6)
C(39)	0.049(5)	0.064(5)	0.092(7)	0.022(4)	0.019(5)	0.008(5)
C(41)	0.027(3)	0.038(3)	0.034(3)	-0.007(2)	0.017(3)	-0.002(2)
C(42)	0.037(3)	0.040(3)	0.043(3)	-0.004(2)	0.027(3)	0.003(3)
C(43)	0.047(4)	0.044(4)	0.049(4)	-0.007(3)	0.030(3)	0.007(3)
C(44)	0.052(4)	0.063(4)	0.048(4)	-0.021(4)	0.034(4)	-0.003(3)
C(45)	0.047(4)	0.062(4)	0.053(4)	-0.009(3)	0.038(4)	-0.008(3)
C(46)	0.035(3)	0.054(4)	0.043(3)	0.007(3)	0.026(3)	0.003(3)
C(51)	0.023(3)	0.056(4)	0.034(3)	0.009(3)	0.016(3)	-0.001(3)
C(52)	0.028(3)	0.066(4)	0.043(4)	-0.011(3)	0.020(3)	-0.014(3)
C(53)	0.039(5)	0.109(7)	0.068(6)	-0.025(4)	0.034(5)	-0.051(5)
C(54)	0.027(4)	0.137(9)	0.039(4)	0.005(5)	0.010(4)	-0.033(5)
C(55)	0.056(6)	0.121(8)	0.040(4)	0.041(5)	0.023(4)	0.012(5)
C(56)	0.035(4)	0.073(5)	0.041(4)	0.016(3)	0.017(3)	0.009(3)

Table S3. Anisotropic thermal parameters for 4. 8cont'd.)

ATOM	U11	U22	U33	U12	U13	U23
C(61)	0.033(3)	0.029(3)	0.031(3)	-0.006(2)	0.019(3)	-0.002(2)
C(62)	0.030(3)	0.029(3)	0.042(3)	-0.002(2)	0.016(3)	-0.006(3)
C(63)	0.031(3)	0.046(4)	0.047(4)	-0.005(3)	0.016(3)	-0.006(3)
C(64)	0.046(4)	0.042(4)	0.047(4)	-0.008(3)	0.018(4)	-0.001(3)
C(65)	0.059(5)	0.027(3)	0.043(3)	-0.005(3)	0.024(3)	-0.006(3)
C(66)	0.044(4)	0.029(3)	0.039(3)	0.002(2)	0.021(3)	0.001(3)
C(71)	0.039(3)	0.031(3)	0.037(3)	0.013(2)	0.025(3)	0.008(2)
C(72)	0.061(5)	0.038(3)	0.051(4)	-0.003(3)	0.039(4)	0.001(3)
C(73)	0.088(7)	0.046(4)	0.075(6)	0.012(4)	0.061(6)	0.016(4)
C(74)	0.086(7)	0.074(5)	0.049(4)	0.034(5)	0.049(5)	0.026(4)
C(75)	0.057(5)	0.076(5)	0.033(3)	0.024(4)	0.026(4)	0.008(3)
C(76)	0.041(4)	0.046(3)	0.037(3)	0.012(3)	0.025(3)	0.003(3)
C(81)	0.25(2)	0.077(8)	0.24(2)	0.05(1)	0.21(2)	0.05(1)
B(1)	0.023(3)	0.027(3)	0.031(3)	-0.003(2)	0.016(3)	-0.003(2)

Table S4. Interatomic distances (Å) and bond angles (deg) for 4.

ATOM	ATOM	DISTANCE	ATOM	ATOM	DISTANCE
Rh(1)	P(1)	2.205(2)	C(11)	C(14)	1.500(9)
Rh(1)	P(2)	2.216(1)	C(12)	C(13)	1.37(1)
Rh(1)	N(11)	2.130(6)	C(13)	C(17)	1.500(7)
Rh(1)	N(21)	2.103(4)	C(14)	C(15)	1.51(1)
Cl(1)	C(81)	1.76(2)	C(14)	C(16)	1.50(1)
Cl(2)	C(81)	1.76(2)	C(17)	C(18)	1.52(2)
P(1)	C(1)	1.818(6)	C(17)	C(19)	1.49(1)
P(1)	C(41)	1.837(9)	C(21)	C(22)	1.405(8)
P(1)	C(51)	1.835(5)	C(21)	C(24)	1.481(7)
P(2)	C(2)	1.821(9)	C(22)	C(23)	1.362(7)
P(2)	C(61)	1.833(5)	C(23)	C(27)	1.509(7)
P(2)	C(71)	1.851(8)	C(24)	C(25)	1.51(2)
N(11)	N(12)	1.383(5)	C(24)	C(26)	1.52(1)
N(11)	C(11)	1.34(1)	C(27)	C(28)	1.54(1)
N(12)	C(13)	1.36(1)	C(27)	C(29)	1.50(2)
N(12)	B(1)	1.55(1)	C(31)	C(32)	1.385(8)
N(21)	N(22)	1.376(5)	C(31)	C(34)	1.50(1)
N(21)	C(21)	1.339(6)	C(32)	C(33)	1.37(1)
N(22)	C(23)	1.362(7)	C(33)	C(37)	1.507(8)
N(22)	B(1)	1.568(7)	C(34)	C(35)	1.51(2)
N(31)	N(32)	1.367(6)	C(34)	C(36)	1.529(9)
N(31)	C(31)	1.33(1)	C(37)	C(38)	1.52(2)
N(32)	C(33)	1.360(9)	C(37)	C(39)	1.49(1)
N(32)	B(1)	1.53(1)	C(41)	C(42)	1.374(8)
C(1)	C(2)	1.33(1)	C(41)	C(46)	1.39(1)
C(11)	C(12)	1.394(9)	C(42)	C(43)	1.39(1)
C(43)	C(44)	1.40(2)	C(63)	C(64)	1.38(1)
C(44)	C(45)	1.38(1)	C(64)	C(65)	1.40(1)
C(45)	C(46)	1.37(1)	C(65)	C(66)	1.396(9)
C(51)	C(52)	1.41(1)	C(71)	C(72)	1.39(1)
C(51)	C(56)	1.38(1)	C(71)	C(76)	1.366(8)
C(52)	C(53)	1.403(9)	C(72)	C(73)	1.40(1)
C(53)	C(54)	1.33(1)	C(73)	C(74)	1.35(1)
C(54)	C(55)	1.43(2)	C(74)	C(75)	1.41(1)
C(55)	C(56)	1.39(1)	C(75)	C(76)	1.37(1)
C(61)	C(62)	1.393(9)	Rh(1)	N(31)	2.893(4)
C(61)	C(66)	1.385(9)	Rh(1)	N(32)	3.497(4)
C(62)	C(63)	1.377(8)			

ATOM	ATOM	ATOM	ANGLE	ATOM	ATOM	ATOM	ANGLE
P(1)	Rh(1)	P(2)	84.57(6)	Rh(1)	P(1)	C(51)	122.7(3)
P(1)	Rh(1)	N(11)	174.7(1)	C(1)	P(1)	C(41)	103.3(4)
P(1)	Rh(1)	N(21)	97.8(2)	C(1)	P(1)	C(51)	98.2(3)
P(2)	Rh(1)	N(11)	97.9(1)	C(41)	P(1)	C(51)	100.3(3)
P(2)	Rh(1)	N(21)	177.5(2)	Rh(1)	P(2)	C(2)	110.3(2)
N(11)	Rh(1)	N(21)	79.7(2)	Rh(1)	P(2)	C(61)	119.3(2)
Rh(1)	P(1)	C(1)	111.0(3)	Rh(1)	P(2)	C(71)	119.8(2)
Rh(1)	P(1)	C(41)	118.1(2)	C(2)	P(2)	C(61)	102.7(3)

Table S4. Interatomic distances (Å) and bond angles (deg) for 4. (cont'd.)

ATOM	ATOM	ATOM	ANGLE	ATOM	ATOM	ATOM	ANGLE
C(2)	P(2)	C(71)	97.9(3)	C(32)	C(33)	C(37)	127.8(7)
C(61)	P(2)	C(71)	103.6(3)	C(31)	C(34)	C(35)	111.4(6)
Rh(1)	N(11)	N(12)	116.2(5)	C(31)	C(34)	C(36)	110.6(6)
Rh(1)	N(11)	C(11)	135.9(4)	C(35)	C(34)	C(36)	110.4(7)
N(12)	N(11)	C(11)	107.0(5)	C(33)	C(37)	C(38)	110.2(8)
N(11)	N(12)	C(13)	108.8(6)	C(33)	C(37)	C(39)	111.3(6)
N(11)	N(12)	B(1)	123.0(5)	C(38)	C(37)	C(39)	110.4(8)
C(13)	N(12)	B(1)	127.1(4)	P(1)	C(41)	C(42)	120.4(7)
Rh(1)	N(21)	N(22)	119.1(3)	P(1)	C(41)	C(46)	120.4(5)
Rh(1)	N(21)	C(21)	133.1(3)	C(42)	C(41)	C(46)	119.3(8)
N(22)	N(21)	C(21)	107.5(4)	C(41)	C(42)	C(43)	120.7(9)
N(21)	N(22)	C(23)	108.6(4)	C(42)	C(43)	C(44)	119.3(6)
N(21)	N(22)	B(1)	122.1(4)	C(43)	C(44)	C(45)	119(1)
C(23)	N(22)	B(1)	128.0(4)	C(44)	C(45)	C(46)	121(1)
N(32)	N(31)	C(31)	105.8(5)	C(41)	C(46)	C(45)	120.6(7)
N(31)	N(32)	C(33)	110.6(6)	P(1)	C(51)	C(52)	120.9(5)
N(31)	N(32)	B(1)	119.6(5)	P(1)	C(51)	C(56)	119.9(5)
C(33)	N(32)	B(1)	129.8(5)	C(52)	C(51)	C(56)	119.0(5)
P(1)	C(1)	C(2)	116.5(7)	C(51)	C(52)	C(53)	119.4(7)
P(2)	C(2)	C(1)	117.1(5)	C(52)	C(53)	C(54)	122(1)
N(11)	C(11)	C(12)	110.0(6)	C(53)	C(54)	C(55)	118.4(7)
N(11)	C(11)	C(14)	121.5(7)	C(54)	C(55)	C(56)	120.4(9)
C(12)	C(11)	C(14)	128.4(9)	C(51)	C(56)	C(55)	120.4(8)
C(11)	C(12)	C(13)	106.0(8)	P(2)	C(61)	C(62)	118.9(4)
N(12)	C(13)	C(12)	108.3(5)	P(2)	C(61)	C(66)	122.6(5)
N(12)	C(13)	C(17)	123.4(7)	C(62)	C(61)	C(66)	118.5(5)
C(12)	C(13)	C(17)	128.1(7)	C(61)	C(62)	C(63)	120.7(6)
C(11)	C(14)	C(15)	111.7(6)	C(62)	C(63)	C(64)	121.6(7)
C(11)	C(14)	C(16)	111.6(5)	C(63)	C(64)	C(65)	118.0(6)
C(15)	C(14)	C(16)	110(1)	C(64)	C(65)	C(66)	120.8(6)
C(13)	C(17)	C(18)	110.8(7)	C(61)	C(66)	C(65)	120.4(7)
C(13)	C(17)	C(19)	111.8(7)	P(2)	C(71)	C(72)	122.8(5)
C(18)	C(17)	C(19)	110.2(7)	P(2)	C(71)	C(76)	117.7(6)
N(21)	C(21)	C(22)	109.0(4)	C(72)	C(71)	C(76)	119.5(7)
N(21)	C(21)	C(24)	123.2(5)	C(71)	C(72)	C(73)	119.2(6)
C(22)	C(21)	C(24)	127.6(5)	C(72)	C(73)	C(74)	121.2(9)
C(21)	C(22)	C(23)	106.3(5)	C(73)	C(74)	C(75)	119.2(9)
N(22)	C(23)	C(22)	108.5(4)	C(74)	C(75)	C(76)	119.5(6)
N(22)	C(23)	C(27)	124.8(4)	C(71)	C(76)	C(75)	121.3(7)
C(22)	C(23)	C(27)	126.7(5)	Cl(1)	C(81)	Cl(2)	111(1)
C(21)	C(24)	C(25)	111.3(7)	N(12)	B(1)	N(22)	107.0(5)
C(21)	C(24)	C(26)	112.0(6)	N(12)	B(1)	N(32)	113.3(4)
C(25)	C(24)	C(26)	110.4(6)	N(22)	B(1)	N(32)	114.1(6)
C(23)	C(27)	C(28)	111.0(6)				
C(23)	C(27)	C(29)	109.9(7)				
C(28)	C(27)	C(29)	110.7(7)				
N(31)	C(31)	C(32)	110.6(6)				
N(31)	C(31)	C(34)	121.3(5)				
C(32)	C(31)	C(34)	128.0(7)				
C(31)	C(32)	C(33)	106.3(7)				
N(32)	C(33)	C(32)	106.7(5)				
N(32)	C(33)	C(37)	125.5(7)				

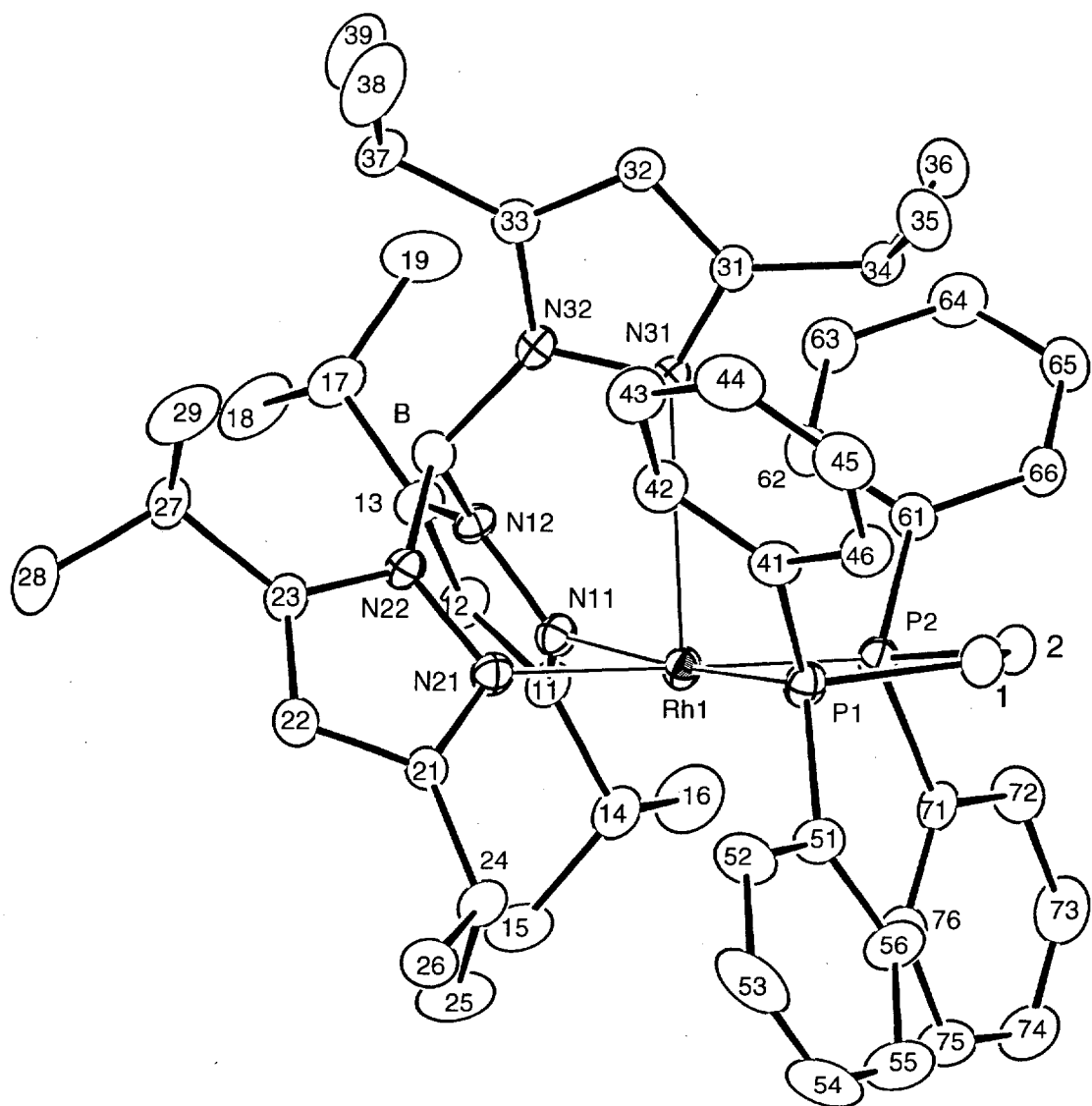


Figure S1. Atomic numbering scheme for **4**.

Labels without atom names are for the carbon atoms.