Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting information

Ru-Pt and Ru-Pd Heterobimetallic Complexes Based on a New Ligand with Two Distinct Chelate Sites

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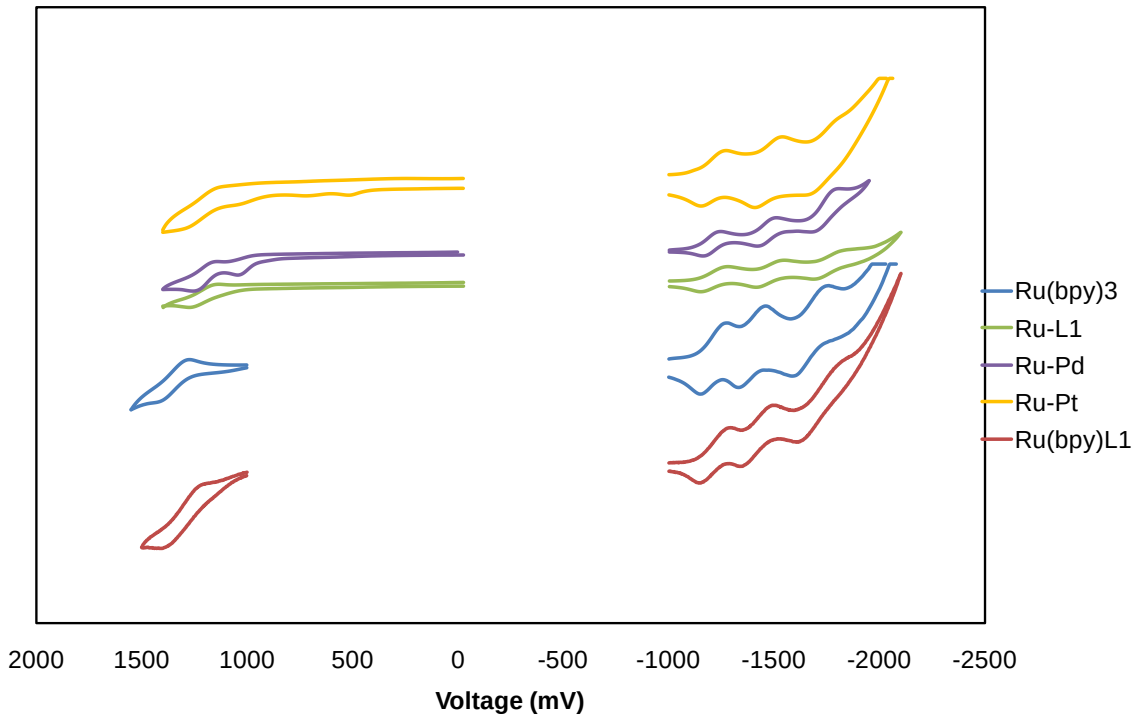

Figure S1. Cyclic voltammogram of metal complexes, recorded in DMF, using NBu_4PF_6 as the electrolyte with a scan rate of 50 -200 mV/s.

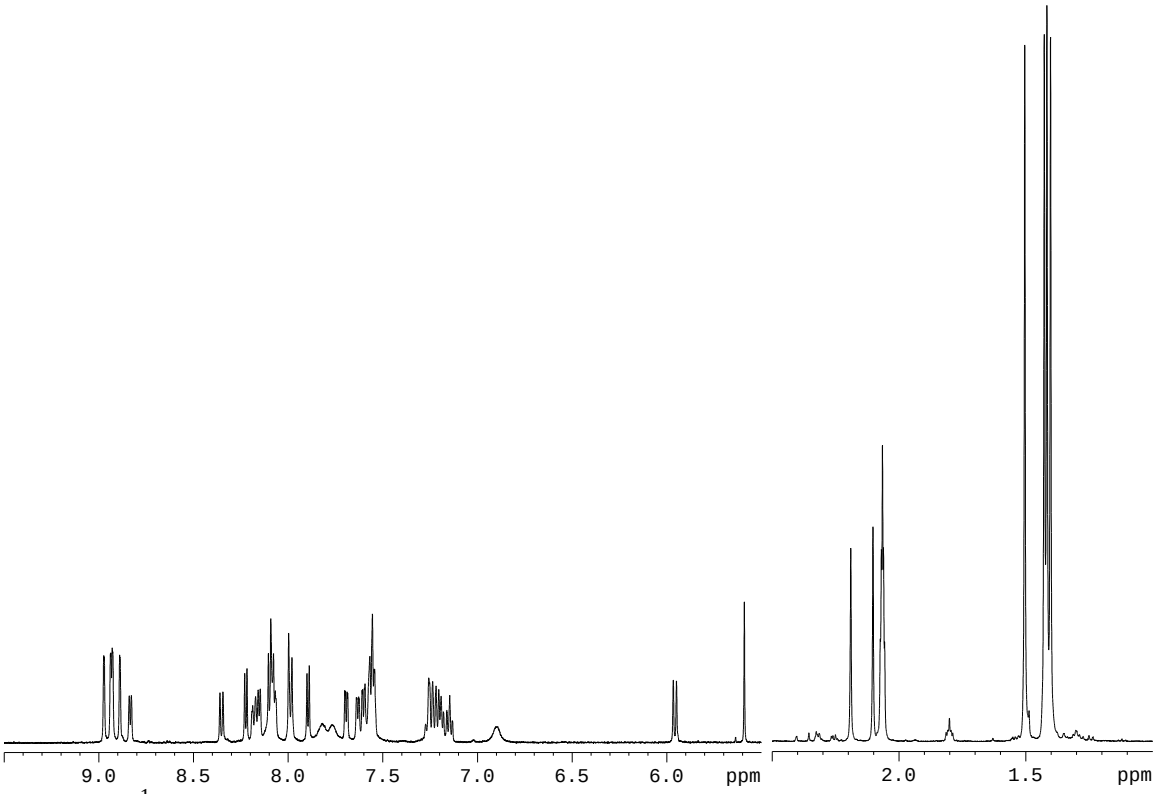

Figure S2. ^{1}H NMR of **Ru-Pd** in Acetone-d_6 at 298K.

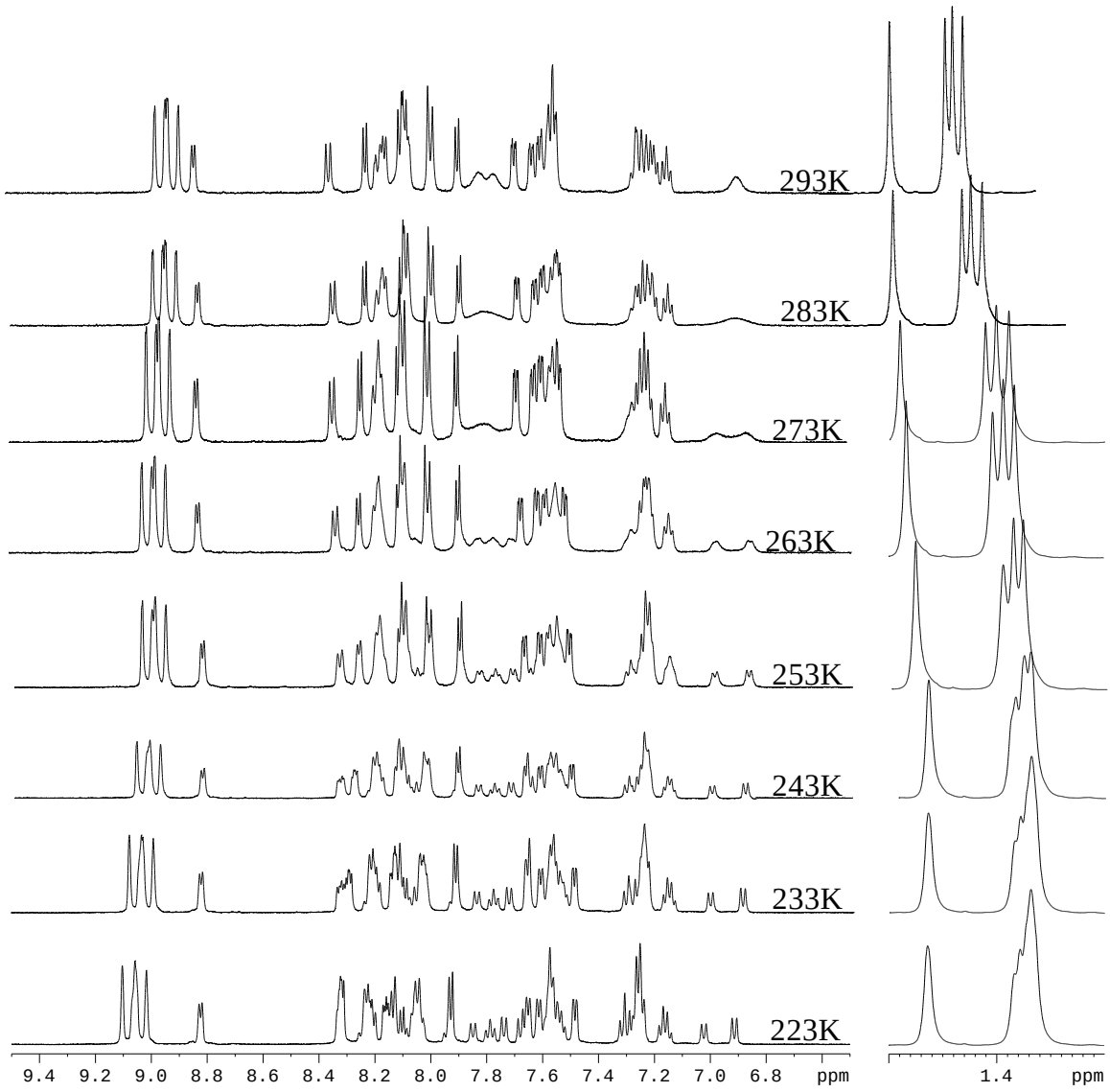

Figure S3. Variable temperature ^{1}H NMR of **Ru-Pd** in Acetone-d_6.

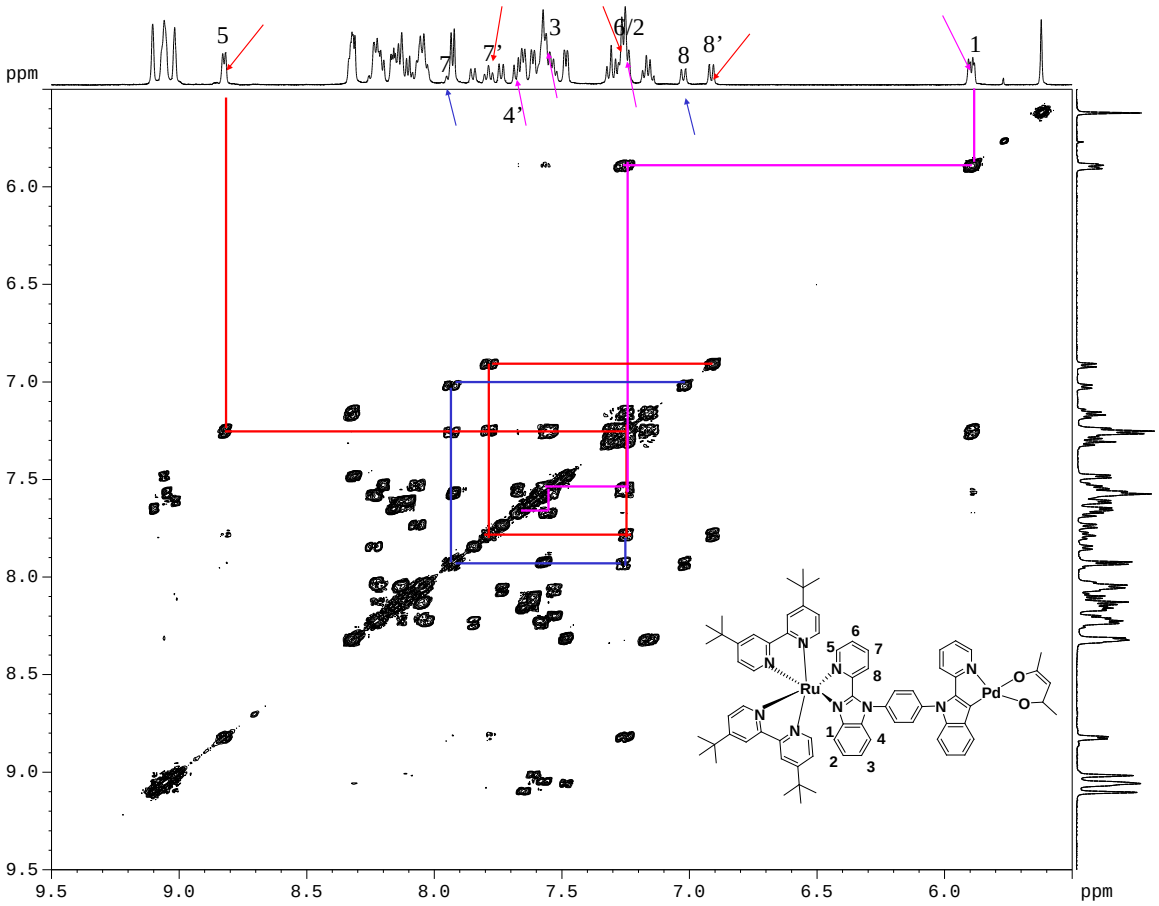

Figure S4. The partial COSY spectrum of **Ru-Pd** in Acetone-d_6 at 223K.

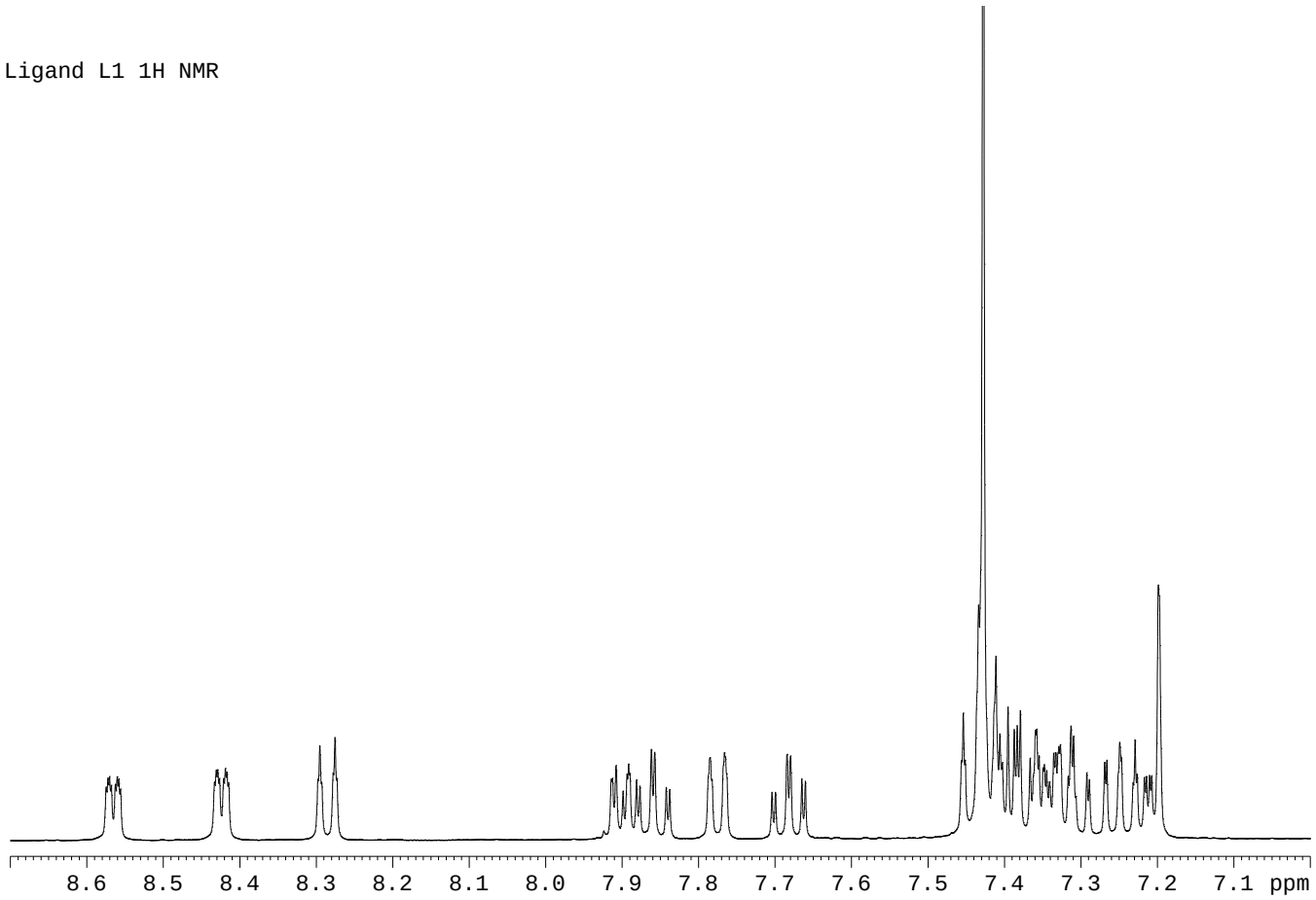

Figure S5. ^{1}H NMR of ligand L1 in CD_2Cl_2.

Table 1. Crystal data and structure refinement for Ligand 1.

Identification code	Ligand 1	
Empirical formula	C31 H21 N5	
Formula weight	463.53	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 7.578(4) Å	α= 90°.
	b = 10.822(5) Å	β= 90°.
	c = 28.380(14) Å	γ = 90°.
Volume	2327(2) $Å^3$	
Z	4	
Density (calculated)	1.323 Mg/m^3	
Absorption coefficient	0.080 mm^{-1}	
F(000)	968	
Crystal size	0.10 x 0.05 x 0.05 mm^3	
Theta range for data collection	1.44 to 24.99°.	
Index ranges	-9<=h<=9, -12<=k<=12, -33<=l<=33	
Reflections collected	20451	
Independent reflections	4078 [R(int) = 0.1040]	
Completeness to theta = 24.99°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9960 and 0.9920	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4078 / 0 / 326	
Goodness-of-fit on F^2	1.147	
Final R indices [I>2sigma(I)]	R1 = 0.0858, wR2 = 0.2113	
R indices (all data)	R1 = 0.0991, wR2 = 0.2200	
Absolute structure parameter	0(5)	
Largest diff. peak and hole	0.480 and -0.371 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Ligand 1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	5855(5)	8705(3)	7361(1)	29(1)
N(2)	9321(5)	8307(4)	7853(1)	34(1)
N(3)	4566(5)	9443(3)	9282(1)	31(1)
N(4)	3692(6)	10253(4)	9972(1)	40(1)
N(5)	940(5)	10017(4)	8966(1)	30(1)
C(1)	4799(6)	9047(4)	6987(2)	31(1)
C(2)	3081(6)	9542(4)	6983(2)	36(1)
C(3)	2393(7)	9800(5)	6552(2)	43(1)
C(4)	3235(8)	9578(5)	6136(2)	49(1)
C(5)	4896(7)	9042(5)	6138(2)	42(1)
C(6)	5679(7)	8763(4)	6567(2)	36(1)
C(7)	7320(6)	8216(4)	6702(2)	32(1)
C(8)	7383(6)	8182(4)	7174(2)	28(1)
C(9)	8834(6)	7700(4)	7467(2)	31(1)
C(10)	9646(7)	6600(4)	7324(2)	38(1)
C(11)	11019(7)	6147(4)	7589(2)	45(1)
C(12)	11514(7)	6744(5)	7987(2)	45(1)
C(13)	10656(7)	7830(5)	8108(2)	40(1)
C(14)	5448(6)	8875(4)	7841(2)	29(1)
C(15)	5549(6)	7906(4)	8159(2)	31(1)
C(16)	5224(6)	8086(4)	8625(2)	30(1)
C(17)	4749(6)	9252(4)	8792(2)	27(1)
C(18)	4610(6)	10225(4)	8474(2)	28(1)
C(19)	4932(5)	10048(4)	8007(2)	26(1)
C(20)	5875(7)	9159(4)	9609(2)	35(1)
C(21)	7489(7)	8536(4)	9568(2)	43(1)
C(22)	8435(9)	8434(5)	9964(2)	57(2)
C(23)	7906(10)	8900(6)	10391(2)	66(2)
C(24)	6320(10)	9518(6)	10436(2)	62(2)
C(25)	5319(8)	9658(5)	10034(2)	42(1)
C(26)	3320(6)	10130(4)	9530(2)	31(1)
C(27)	1648(7)	10605(4)	9331(2)	32(1)

C(28)	896(7)	11656(5)	9535(2)	43(1)
C(29)	-649(7)	12095(5)	9351(2)	44(1)
C(30)	-1410(7)	11498(5)	8979(2)	41(1)
C(31)	-582(6)	10460(4)	8800(2)	35(1)

Table 3. Bond lengths [Å] and angles [°] for Ligand 1.

N(1)-C(1)	1.380(6)	C(11)-C(12)	1.354(8)
N(1)-C(8)	1.394(6)	C(11)-H(11A)	0.9500
N(1)-C(14)	1.409(6)	C(12)-C(13)	1.386(7)
N(2)-C(9)	1.330(6)	C(12)-H(12A)	0.9500
N(2)-C(13)	1.348(6)	C(13)-H(13A)	0.9500
N(3)-C(20)	1.393(6)	C(14)-C(15)	1.386(6)
N(3)-C(26)	1.393(6)	C(14)-C(19)	1.410(6)
N(3)-C(17)	1.414(6)	C(15)-C(16)	1.359(6)
N(4)-C(26)	1.293(6)	C(15)-H(15A)	0.9500
N(4)-C(25)	1.402(7)	C(16)-C(17)	1.395(6)
N(5)-C(27)	1.327(6)	C(16)-H(16A)	0.9500
N(5)-C(31)	1.336(6)	C(17)-C(18)	1.391(6)
C(1)-C(6)	1.400(7)	C(18)-C(19)	1.359(6)
C(1)-C(2)	1.408(7)	C(18)-H(18A)	0.9500
C(2)-C(3)	1.360(7)	C(19)-H(19A)	0.9500
C(2)-H(2A)	0.9500	C(20)-C(25)	1.385(7)
C(3)-C(4)	1.362(8)	C(20)-C(21)	1.402(7)
C(3)-H(3A)	0.9500	C(21)-C(22)	1.338(8)
C(4)-C(5)	1.386(8)	C(21)-H(21A)	0.9500
C(4)-H(4A)	0.9500	C(22)-C(23)	1.374(9)
C(5)-C(6)	1.387(7)	C(22)-H(22A)	0.9500
C(5)-H(5A)	0.9500	C(23)-C(24)	1.381(10)
C(6)-C(7)	1.430(7)	C(23)-H(23A)	0.9500
C(7)-C(8)	1.338(7)	C(24)-C(25)	1.378(8)
C(7)-H(7A)	0.9500	C(24)-H(24A)	0.9500
C(8)-C(9)	1.474(7)	C(26)-C(27)	1.480(7)
C(9)-C(10)	1.399(6)	C(27)-C(28)	1.398(7)
C(10)-C(11)	1.375(7)	C(28)-C(29)	1.367(7)
C(10)-H(10A)	0.9500	C(28)-H(28A)	0.9500

C(29)-C(30)	1.366(7)	C(7)-C(8)-N(1)	109.9(4)
C(29)-H(29A)	0.9500	C(7)-C(8)-C(9)	126.9(4)
C(30)-C(31)	1.384(7)	N(1)-C(8)-C(9)	123.2(4)
C(30)-H(30A)	0.9500	N(2)-C(9)-C(10)	122.5(5)
C(31)-H(31A)	0.9500	N(2)-C(9)-C(8)	119.8(4)
		C(10)-C(9)-C(8)	117.7(4)
C(1)-N(1)-C(8)	107.3(4)	C(11)-C(10)-C(9)	118.5(5)
C(1)-N(1)-C(14)	125.6(4)	C(11)-C(10)-H(10A)	120.7
C(8)-N(1)-C(14)	127.2(4)	C(9)-C(10)-H(10A)	120.7
C(9)-N(2)-C(13)	117.6(4)	C(12)-C(11)-C(10)	119.7(5)
C(20)-N(3)-C(26)	105.3(4)	C(12)-C(11)-H(11A)	120.1
C(20)-N(3)-C(17)	123.7(4)	C(10)-C(11)-H(11A)	120.1
C(26)-N(3)-C(17)	129.9(4)	C(11)-C(12)-C(13)	118.8(5)
C(26)-N(4)-C(25)	105.4(4)	C(11)-C(12)-H(12A)	120.6
C(27)-N(5)-C(31)	116.9(4)	C(13)-C(12)-H(12A)	120.6
N(1)-C(1)-C(6)	108.7(4)	N(2)-C(13)-C(12)	122.9(5)
N(1)-C(1)-C(2)	130.1(4)	N(2)-C(13)-H(13A)	118.6
C(6)-C(1)-C(2)	121.2(4)	C(12)-C(13)-H(13A)	118.6
C(3)-C(2)-C(1)	116.0(5)	C(15)-C(14)-N(1)	121.3(4)
C(3)-C(2)-H(2A)	122.0	C(15)-C(14)-C(19)	118.6(4)
C(1)-C(2)-H(2A)	122.0	N(1)-C(14)-C(19)	120.1(4)
C(2)-C(3)-C(4)	124.3(5)	C(16)-C(15)-C(14)	121.0(4)
C(2)-C(3)-H(3A)	117.8	C(16)-C(15)-H(15A)	119.5
C(4)-C(3)-H(3A)	117.8	C(14)-C(15)-H(15A)	119.5
C(3)-C(4)-C(5)	119.7(5)	C(15)-C(16)-C(17)	120.4(4)
C(3)-C(4)-H(4A)	120.1	C(15)-C(16)-H(16A)	119.8
C(5)-C(4)-H(4A)	120.1	C(17)-C(16)-H(16A)	119.8
C(4)-C(5)-C(6)	118.9(5)	C(18)-C(17)-C(16)	119.0(4)
C(4)-C(5)-H(5A)	120.6	C(18)-C(17)-N(3)	121.4(4)
C(6)-C(5)-H(5A)	120.6	C(16)-C(17)-N(3)	119.4(4)
C(5)-C(6)-C(1)	119.7(5)	C(19)-C(18)-C(17)	120.8(4)
C(5)-C(6)-C(7)	134.3(5)	C(19)-C(18)-H(18A)	119.6
C(1)-C(6)-C(7)	106.0(4)	C(17)-C(18)-H(18A)	119.6
C(8)-C(7)-C(6)	108.1(4)	C(18)-C(19)-C(14)	120.2(4)
C(8)-C(7)-H(7A)	125.9	C(18)-C(19)-H(19A)	119.9
C(6)-C(7)-H(7A)	125.9	C(14)-C(19)-H(19A)	119.9

C(25)-C(20)-N(3)	106.1(4)	N(4)-C(26)-N(3)	113.4(4)
C(25)-C(20)-C(21)	121.8(5)	N(4)-C(26)-C(27)	121.5(4)
N(3)-C(20)-C(21)	132.1(5)	N(3)-C(26)-C(27)	124.9(4)
C(22)-C(21)-C(20)	115.8(5)	N(5)-C(27)-C(28)	123.3(5)
C(22)-C(21)-H(21A)	122.1	N(5)-C(27)-C(26)	118.5(4)
C(20)-C(21)-H(21A)	122.1	C(28)-C(27)-C(26)	118.2(4)
C(21)-C(22)-C(23)	123.8(6)	C(29)-C(28)-C(27)	118.2(5)
C(21)-C(22)-H(22A)	118.1	C(29)-C(28)-H(28A)	120.9
C(23)-C(22)-H(22A)	118.1	C(27)-C(28)-H(28A)	120.9
C(22)-C(23)-C(24)	120.8(5)	C(30)-C(29)-C(28)	119.6(5)
C(22)-C(23)-H(23A)	119.6	C(30)-C(29)-H(29A)	120.2
C(24)-C(23)-H(23A)	119.6	C(28)-C(29)-H(29A)	120.2
C(25)-C(24)-C(23)	117.2(6)	C(29)-C(30)-C(31)	118.4(5)
C(25)-C(24)-H(24A)	121.4	C(29)-C(30)-H(30A)	120.8
C(23)-C(24)-H(24A)	121.4	C(31)-C(30)-H(30A)	120.8
C(24)-C(25)-C(20)	120.6(5)	N(5)-C(31)-C(30)	123.6(5)
C(24)-C(25)-N(4)	129.6(5)	N(5)-C(31)-H(31A)	118.2
C(20)-C(25)-N(4)	109.8(4)	C(30)-C(31)-H(31A)	118.2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Ligand 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	26(2)	23(2)	37(2)	-2(2)	0(2)	-2(2)
N(2)	31(2)	27(2)	43(2)	-2(2)	-2(2)	3(2)
N(3)	33(2)	26(2)	36(2)	1(2)	-4(2)	1(2)
N(4)	43(3)	36(2)	41(2)	-6(2)	-1(2)	4(2)
N(5)	20(2)	31(2)	40(2)	-4(2)	1(2)	2(2)
C(1)	32(3)	24(2)	38(3)	0(2)	-1(2)	-9(2)
C(2)	33(3)	24(2)	52(3)	-3(2)	1(2)	-1(2)
C(3)	38(3)	36(3)	55(3)	0(2)	-14(2)	-5(2)
C(4)	57(4)	42(3)	48(3)	6(2)	-17(3)	-15(3)
C(5)	47(3)	36(3)	43(3)	-2(2)	-1(2)	-14(2)
C(6)	46(3)	23(2)	39(3)	-1(2)	2(2)	-15(2)

C(7)	30(3)	25(2)	41(3)	-6(2)	5(2)	-4(2)
C(8)	22(2)	18(2)	45(3)	-4(2)	4(2)	1(2)
C(9)	19(2)	27(2)	45(3)	-2(2)	7(2)	0(2)
C(10)	31(3)	23(2)	61(3)	-11(2)	2(2)	3(2)
C(11)	26(3)	22(2)	87(4)	-6(2)	8(3)	7(2)
C(12)	31(3)	30(3)	73(4)	2(3)	-7(3)	5(2)
C(13)	30(3)	33(3)	57(3)	-3(2)	-8(2)	-4(2)
C(14)	27(2)	18(2)	41(2)	2(2)	-1(2)	-3(2)
C(15)	33(3)	13(2)	49(3)	1(2)	4(2)	-3(2)
C(16)	26(2)	19(2)	44(3)	5(2)	3(2)	2(2)
C(17)	19(2)	22(2)	40(2)	2(2)	2(2)	1(2)
C(18)	23(2)	18(2)	41(3)	-2(2)	0(2)	-1(2)
C(19)	20(2)	19(2)	40(3)	1(2)	-2(2)	-1(2)
C(20)	34(3)	27(2)	44(3)	4(2)	-8(2)	-3(2)
C(21)	45(3)	21(2)	62(3)	5(2)	-5(3)	4(2)
C(22)	58(4)	40(3)	72(4)	5(3)	-24(3)	6(3)
C(23)	82(5)	43(3)	73(4)	-1(3)	-45(4)	8(3)
C(24)	85(5)	49(4)	50(3)	-6(3)	-19(3)	15(4)
C(25)	52(3)	33(3)	40(3)	-1(2)	-11(2)	-1(2)
C(26)	32(2)	24(2)	37(3)	-2(2)	4(2)	-1(2)
C(27)	33(3)	28(2)	36(2)	-5(2)	4(2)	1(2)
C(28)	44(3)	38(3)	48(3)	-8(2)	0(2)	8(2)
C(29)	42(3)	38(3)	52(3)	-8(2)	3(2)	12(3)
C(30)	35(3)	33(3)	55(3)	1(2)	2(2)	7(2)
C(31)	24(2)	34(3)	46(3)	-2(2)	0(2)	1(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for Ligand 1.

	x	y	z	U(eq)
H(2A)	2440	9688	7266	44
H(3A)	1249	10158	6539	52
H(4A)	2686	9790	5846	59
H(5A)	5488	8868	5851	50
H(7A)	8211	7927	6494	38
H(10A)	9257	6177	7049	46
H(11A)	11617	5417	7494	54
H(12A)	12433	6425	8179	53
H(13A)	11026	8256	8384	48
H(15A)	5851	7104	8050	38
H(16A)	5321	7414	8839	36
H(18A)	4286	11023	8584	33
H(19A)	4809	10717	7793	32
H(21A)	7887	8207	9276	51
H(22A)	9535	8014	9949	68
H(23A)	8641	8797	10660	80
H(24A)	5935	9833	10731	74
H(28A)	1444	12055	9795	52
H(29A)	-1190	12809	9481	53
H(30A)	-2483	11790	8846	49
H(31A)	-1126	10039	8544	41

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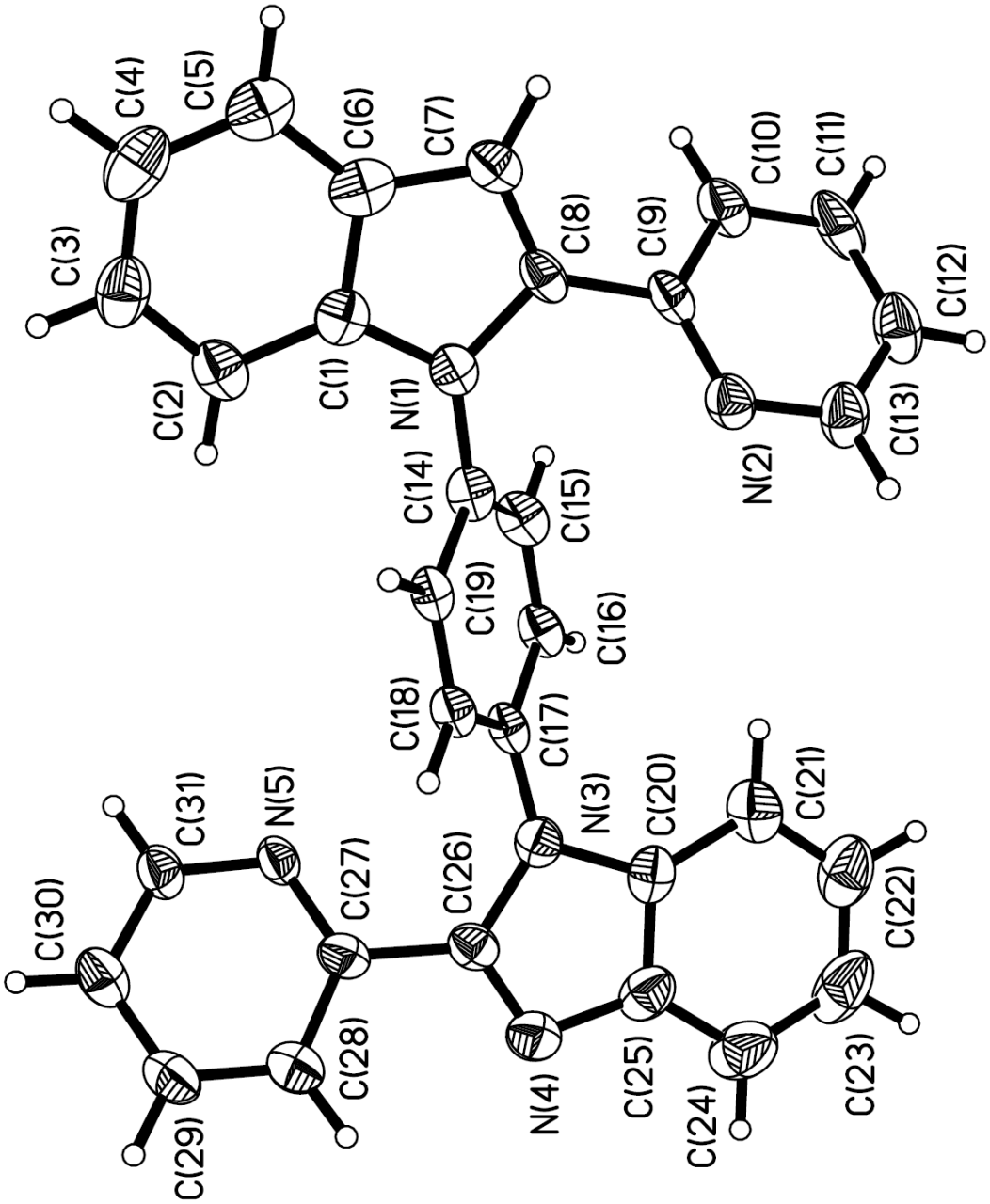


The structure of L1 with labeling schemes and 50% thermal ellipsoids.

Table 1. Crystal data and structure refinement for Pd1.

Identification code	Pd1	
Empirical formula	C24 H20 N2 O2 Pd	
Formula weight	474.82	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 12.1096(18) Å	α= 90°.
	b = 12.2832(18) Å	β= 90°.
	c = 13.777(2) Å	γ = 90°.
Volume	2049.2(5) $Å^3$	
Z	4	
Density (calculated)	1.539 Mg/m^3	
Absorption coefficient	0.928 mm^{-1}	
F(000)	960	
Crystal size	0.20 x 0.20 x 0.20 mm^3	
Theta range for data collection	2.22 to 26.00°.	
Index ranges	-14<=h<=12, -14<=k<=15, -16<=l<=16	
Reflections collected	10916	
Independent reflections	4022 [R(int) = 0.0534]	
Completeness to theta = 26.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8362 and 0.8362	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4022 / 0 / 265	
Goodness-of-fit on F^2	1.074	
Final R indices [I>2sigma(I)]	R1 = 0.0497, wR2 = 0.1159	
R indices (all data)	R1 = 0.0720, wR2 = 0.1316	
Absolute structure parameter	0.24(6)	
Largest diff. peak and hole	2.943 and -0.924 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Pd1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	3817(1)	4748(1)	8587(1)	34(1)
O(1)	2782(4)	3694(5)	7853(3)	45(1)
O(2)	3317(4)	6040(4)	7825(3)	42(1)
N(1)	6039(5)	5667(5)	10656(4)	37(1)
N(2)	4472(5)	3527(5)	9416(4)	37(1)
C(1)	5335(6)	5014(5)	10107(4)	35(2)
C(2)	4820(6)	5616(5)	9402(4)	34(2)
C(3)	5196(6)	6703(6)	9501(5)	35(2)
C(4)	5005(6)	7692(6)	9007(5)	39(2)
C(5)	5519(7)	8611(6)	9298(6)	49(2)
C(6)	6247(8)	8600(6)	10113(6)	54(2)
C(7)	6462(6)	7673(6)	10609(5)	48(2)
C(8)	5952(5)	6720(5)	10300(4)	32(2)
C(9)	5219(6)	3837(6)	10112(5)	40(2)
C(10)	5746(7)	3062(7)	10654(6)	47(2)
C(11)	5518(7)	1965(7)	10497(6)	56(2)
C(12)	4775(8)	1668(7)	9791(6)	60(2)
C(13)	4273(7)	2474(6)	9270(6)	49(2)
C(14)	6557(6)	5391(6)	11565(4)	39(2)
C(15)	7682(6)	5400(7)	11634(5)	51(2)
C(16)	8168(7)	5121(8)	12531(6)	61(2)
C(17)	7527(8)	4828(8)	13298(6)	62(2)
C(18)	6393(8)	4788(7)	13214(5)	59(2)
C(19)	5906(6)	5105(7)	12352(5)	47(2)
C(20)	1608(8)	3076(7)	6626(7)	62(2)
C(21)	2232(6)	3994(7)	7095(5)	43(2)
C(22)	2171(6)	5023(6)	6723(5)	41(2)
C(23)	2660(6)	5961(7)	7078(5)	41(2)
C(24)	2435(8)	7054(7)	6601(6)	60(2)

Table 3. Bond lengths [Å] and angles [°] for Pd1.

Pd(1)-C(2)	1.968(7)		
Pd(1)-O(2)	1.997(5)	C(2)-Pd(1)-O(2)	93.2(2)
Pd(1)-N(2)	2.045(6)	C(2)-Pd(1)-N(2)	80.8(3)
Pd(1)-O(1)	2.066(5)	O(2)-Pd(1)-N(2)	173.7(2)
O(1)-C(21)	1.292(8)	C(2)-Pd(1)-O(1)	173.3(2)
O(2)-C(23)	1.304(8)	O(2)-Pd(1)-O(1)	93.2(2)
N(1)-C(8)	1.388(9)	N(2)-Pd(1)-O(1)	92.8(2)
N(1)-C(1)	1.394(8)	C(21)-O(1)-Pd(1)	122.0(5)
N(1)-C(14)	1.440(8)	C(23)-O(2)-Pd(1)	122.8(5)
N(2)-C(13)	1.331(9)	C(8)-N(1)-C(1)	107.4(5)
N(2)-C(9)	1.372(9)	C(8)-N(1)-C(14)	124.0(5)
C(1)-C(2)	1.371(9)	C(1)-N(1)-C(14)	127.1(6)
C(1)-C(9)	1.453(10)	C(13)-N(2)-C(9)	119.6(7)
C(2)-C(3)	1.418(10)	C(13)-N(2)-Pd(1)	123.9(5)
C(3)-C(4)	1.412(10)	C(9)-N(2)-Pd(1)	116.3(5)
C(3)-C(8)	1.432(9)	C(2)-C(1)-N(1)	110.6(6)
C(4)-C(5)	1.351(11)	C(2)-C(1)-C(9)	119.8(6)
C(5)-C(6)	1.427(12)	N(1)-C(1)-C(9)	129.0(6)
C(6)-C(7)	1.353(11)	C(1)-C(2)-C(3)	107.1(6)
C(7)-C(8)	1.389(10)	C(1)-C(2)-Pd(1)	113.1(5)
C(9)-C(10)	1.368(11)	C(3)-C(2)-Pd(1)	139.8(5)
C(10)-C(11)	1.392(12)	C(4)-C(3)-C(2)	135.3(7)
C(11)-C(12)	1.374(12)	C(4)-C(3)-C(8)	117.6(6)
C(12)-C(13)	1.366(11)	C(2)-C(3)-C(8)	107.1(6)
C(14)-C(15)	1.366(10)	C(5)-C(4)-C(3)	120.0(7)
C(14)-C(19)	1.386(10)	C(4)-C(5)-C(6)	120.7(7)
C(15)-C(16)	1.410(11)	C(7)-C(6)-C(5)	121.6(7)
C(16)-C(17)	1.360(12)	C(6)-C(7)-C(8)	118.0(7)
C(17)-C(18)	1.380(13)	N(1)-C(8)-C(7)	130.1(6)
C(18)-C(19)	1.381(10)	N(1)-C(8)-C(3)	107.8(6)
C(20)-C(21)	1.504(11)	C(7)-C(8)-C(3)	122.1(6)
C(21)-C(22)	1.365(11)	C(10)-C(9)-N(2)	119.7(7)
C(22)-C(23)	1.385(11)	C(10)-C(9)-C(1)	130.5(7)
C(23)-C(24)	1.520(11)	N(2)-C(9)-C(1)	109.7(6)

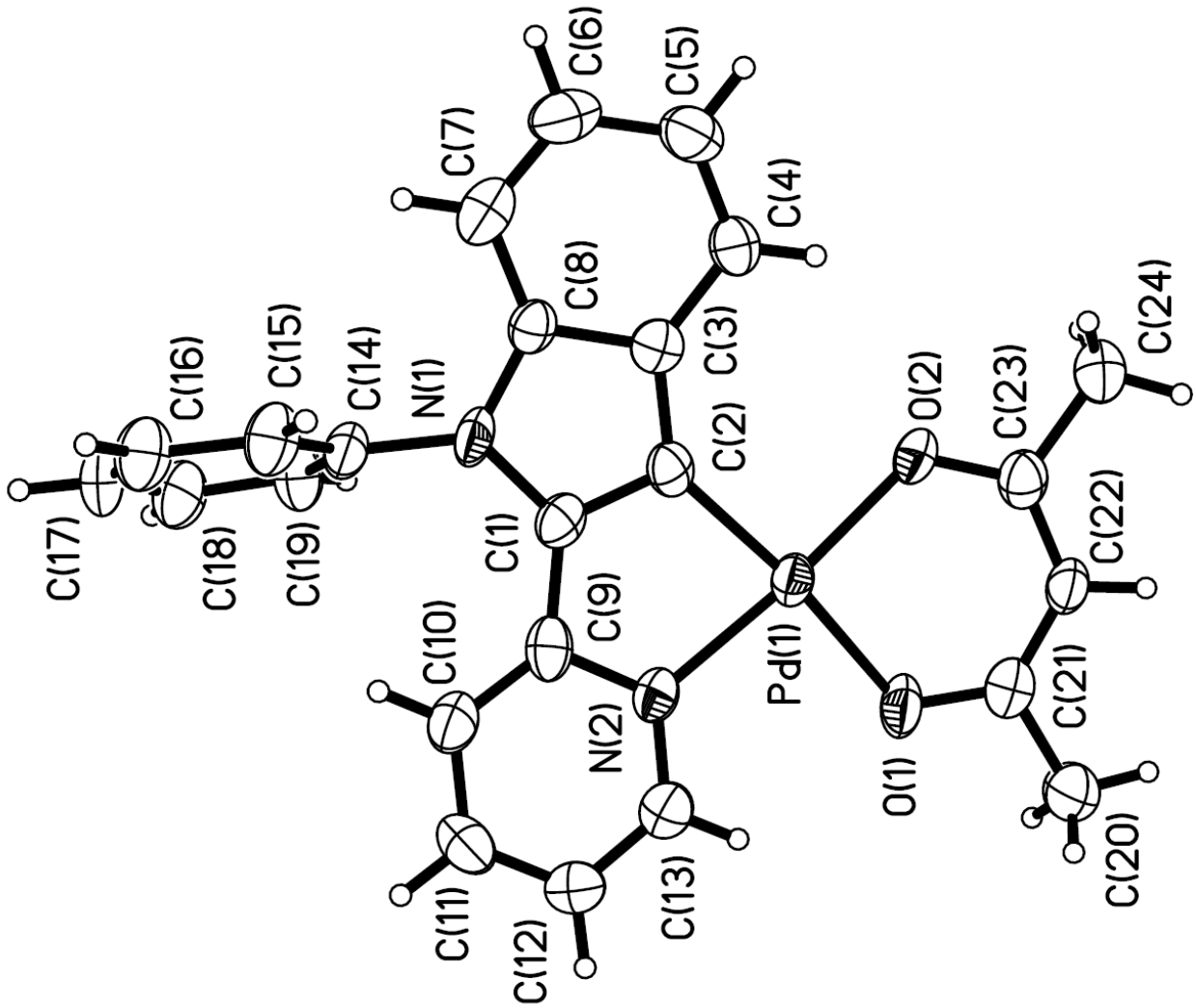
C(9)-C(10)-C(11)	119.8(7)
C(12)-C(11)-C(10)	119.7(8)
C(13)-C(12)-C(11)	118.1(8)
N(2)-C(13)-C(12)	123.0(7)
C(15)-C(14)-C(19)	120.9(6)
C(15)-C(14)-N(1)	119.6(6)
C(19)-C(14)-N(1)	119.5(6)
C(14)-C(15)-C(16)	118.4(7)
C(17)-C(16)-C(15)	120.5(8)
C(16)-C(17)-C(18)	120.8(7)
C(17)-C(18)-C(19)	119.2(8)
C(18)-C(19)-C(14)	120.1(7)
O(1)-C(21)-C(22)	126.5(7)
O(1)-C(21)-C(20)	113.1(7)
C(22)-C(21)-C(20)	120.4(6)
C(21)-C(22)-C(23)	127.9(6)
O(2)-C(23)-C(22)	127.0(7)
O(2)-C(23)-C(24)	112.7(7)
C(22)-C(23)-C(24)	120.4(7)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Pd1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	37(1)	39(1)	25(1)	-2(1)	-4(1)	0(1)
O(1)	47(3)	58(3)	31(2)	2(2)	-15(2)	-4(3)
O(2)	47(3)	44(3)	36(2)	-6(2)	-18(2)	-2(2)
N(1)	43(3)	48(3)	21(2)	-4(2)	-9(3)	-4(3)
N(2)	44(3)	42(3)	25(3)	-3(2)	-2(2)	0(3)
C(1)	39(4)	42(5)	25(3)	-4(3)	5(3)	-3(3)
C(2)	38(4)	40(4)	24(3)	1(3)	4(3)	4(3)
C(3)	33(4)	39(4)	33(3)	-2(3)	4(3)	2(3)
C(4)	34(4)	44(4)	39(4)	3(3)	-4(3)	4(3)
C(5)	57(5)	38(4)	53(4)	5(4)	1(4)	4(4)
C(6)	63(5)	41(4)	59(5)	-8(3)	4(5)	-13(5)
C(7)	42(5)	62(5)	39(4)	-9(4)	-2(3)	-9(4)
C(8)	34(4)	38(4)	25(3)	-5(3)	2(3)	2(3)
C(9)	36(4)	57(5)	26(3)	4(3)	1(3)	-2(4)
C(10)	54(5)	52(5)	35(4)	-6(4)	-9(4)	2(4)
C(11)	73(6)	45(5)	52(5)	10(4)	-9(4)	14(4)
C(12)	90(7)	36(4)	53(5)	-3(4)	-14(5)	-1(5)
C(13)	63(5)	44(4)	40(4)	-2(3)	-7(4)	-3(4)
C(14)	41(3)	43(4)	32(3)	-5(3)	-11(3)	1(3)
C(15)	39(4)	67(6)	48(4)	-2(4)	-10(3)	-3(4)
C(16)	45(4)	67(6)	72(6)	-2(5)	-25(4)	-1(4)
C(17)	81(6)	63(5)	44(4)	6(4)	-33(4)	2(5)
C(18)	80(6)	65(5)	33(3)	-6(4)	-9(4)	4(5)
C(19)	44(4)	65(5)	32(3)	5(3)	-1(3)	4(4)
C(20)	73(6)	49(5)	64(6)	4(4)	-28(5)	-7(4)
C(21)	40(4)	52(5)	36(4)	-2(4)	-4(3)	-1(4)
C(22)	48(4)	45(5)	32(3)	-6(3)	-14(3)	9(3)
C(23)	43(4)	48(5)	32(3)	-3(3)	0(3)	8(4)
C(24)	82(6)	54(5)	45(5)	0(4)	-20(5)	7(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for Pd1.

	x	y	z	U(eq)
H(4A)	4524	7711	8480	47
H(5A)	5398	9259	8965	59
H(6A)	6581	9245	10309	65
H(7A)	6936	7673	11139	57
H(10A)	6255	3267	11125	57
H(11A)	5866	1435	10870	68
H(12A)	4619	939	9672	72
H(13A)	3769	2279	8791	59
H(15A)	8117	5585	11103	61
H(16A)	8932	5139	12598	74
H(17A)	7858	4651	13887	75
H(18A)	5961	4552	13731	71
H(19A)	5141	5126	12300	56
H(20A)	2121	2550	6376	93
H(20B)	1165	3356	6105	93
H(20C)	1139	2735	7099	93
H(22A)	1750	5103	6163	50
H(24A)	3114	7453	6542	90
H(24B)	1924	7461	6991	90
H(24C)	2125	6939	5968	90



The structure of Pd1 with labeling schemes and 50% thermal ellipsoids.