Light-Emitting Cyclopalladated Complexes of 6-Phenyl-2,2'-bipyridines with Hydrogen Bonding Functionality

Francesco Neve,* Alessandra Crispini, Cinzia Di Pietro and Sebastiano Campagna*

Dipartimento di Chimica, Università della Calabria, I-87030 Arcavacata di Rende (CS), Italy, and Dipartimento di Chimica Inorganica, Chimica Analitica e Chimica Fisica, Università di Messina, via Sperone 31, I-98166 Messina, Italy

SUPPORTING INFORMATION

Table S1. Crystal data and structure refinement for [Pd(L1)Cl] (**1**) (1 page).

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **1** (1 page).

Table S3. Bond lengths [Å] and angles [deg] for **1** (2 pages).

Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for **1** (1 page).

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **1** (1 page).

Table S6. Torsion angles [deg] for **1** (2 pages).

Table S7. Hydrogen bond parameters for **1** [Å and deg] (1 page).

Table S1. Crystal data and structure refinement for [Pd(L1)Cl](1).

Empirical formula	C17 H13 Cl N2 O3 Pd
Formula weight	435.14
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 7.9364(16) Å alpha = 111.05(3) deg. b = 9.4593(19) Å beta = 94.59(3) deg. c = 11.247(2) Å gamma = 98.40(3) deg.
Volume	771.5(3) $Å^3$
Z, Calculated density	2, 1.873 Mg/m^3
Absorption coefficient	1.394 mm^{-1}
F(000)	432
Crystal size	0.44 x 0.26 x 0.12 mm
Theta range for data collection	1.96 to 24.05 deg.
Limiting indices	$0 \le h \le 9$, $-10 \le k \le 10$, $-12 \le l \le 12$
Reflections collected / unique	2634 / 2435 [R(int) = 0.0288]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2435 / 3 / 223
Goodness-of-fit on F^2	1.114
Final R indices [I>2sigma(I)]	R1 = 0.0286, wR2 = 0.0762
R indices (all data)	R1 = 0.0299, wR2 = 0.0771
Largest diff. peak and hole	0.555 and -1.109 e. $Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^3$ x 10^3) for **1**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd	6812(1)	5565(1)	4563(1)	30(1)
Cl	5322(1)	6010(1)	2896(1)	41(1)
O(1)	11442(3)	3380(3)	8806(2)	41(1)
O(2)	12184(4)	5935(3)	9789(3)	50(1)
O(3)	14122(4)	3244(4)	10193(3)	57(1)
N(1)	7085(4)	3203(3)	3648(3)	34(1)
N(2)	8154(4)	5256(3)	5964(3)	31(1)
C(1)	6502(5)	2200(4)	2433(4)	40(1)
C(2)	6788(6)	714(5)	1999(4)	48(1)
C(3)	7686(5)	217(4)	2822(4)	48(1)
C(4)	8304(5)	1232(4)	4066(4)	43(1)
C(5)	7991(4)	2715(4)	4453(3)	31(1)
C(6)	8608(4)	3882(4)	5763(3)	29(1)
C(7)	9609(4)	3686(4)	6740(3)	33(1)
C(8)	10116(4)	4904(4)	7910(3)	32(1)
C(9)	9597(4)	6302(4)	8099(3)	34(1)
C(10)	8600(4)	6467(4)	7112(3)	31(1)
C(11)	11345(5)	4799(4)	8939(3)	36(1)
C(12)	7082(4)	7684(4)	5902(4)	34(1)
C(13)	7956(4)	7833(4)	7085(3)	34(1)
C(14)	8233(5)	9221(4)	8143(4)	43(1)
C(15)	7682(5)	10491(4)	8019(4)	50(1)
C(16)	6837(5)	10361(4)	6853(4)	48(1)
C(17)	6532(5)	8985(4)	5805(4)	41(1)

Table S3. Bond lengths [Å] and angles [deg] for **1**.

Pd-N(2)	1.964(3)
Pd-C(12)	1.997(4)
Pd-N(1)	2.150(3)
Pd-Cl	2.3340(11)
O(1)-C(11)	1.311(4)
O(2)-C(11)	1.210(5)
N(1)-C(1)	1.349(5)
N(1)-C(5)	1.358(5)
N(2)-C(6)	1.345(4)
N(2)-C(10)	1.360(5)
C(1)-C(2)	1.372(6)
C(2)-C(3)	1.375(6)
C(3)-C(4)	1.382(6)
C(4)-C(5)	1.378(5)
C(5)-C(6)	1.479(5)
C(6)-C(7)	1.388(5)
C(7)-C(8)	1.383(5)
C(8)-C(9)	1.390(5)
C(8)-C(11)	1.493(5)
C(9)-C(10)	1.380(5)
C(10)-C(13)	1.467(5)
C(12)-C(13)	1.400(5)
C(12)-C(17)	1.402(5)
C(13)-C(14)	1.393(5)
C(14)-C(15)	1.385(5)
C(16)-C(17)	1.379(6)
C(16)-C(15)	1.380(6)
N(2)-Pd-C(12)	81.44(13)
N(2)-Pd-N(1)	78.59(12)
C(12)-Pd-N(1)	159.98(14)
N(2)-Pd-Cl	177.45(8)
C(12)-Pd-Cl	97.45(11)
N(1)-Pd-Cl	102.45(9)
C(1)-N(1)-C(5)	118.3(3)
C(1)-N(1)-Pd	129.4(3)
C(5)-N(1)-Pd	112.2(2)
C(6)-N(2)-C(10)	122.5(3)
C(6)-N(2)-Pd	119.7(2)
C(10)-N(2)-Pd	117.8(2)
N(1)-C(1)-C(2)	122.0(4)
C(1)-C(2)-C(3)	119.5(4)
C(2)-C(3)-C(4)	119.2(4)
C(5)-C(4)-C(3)	119.0(4)
N(1)-C(5)-C(4)	121.8(3)
N(1)-C(5)-C(6)	115.3(3)
C(4)-C(5)-C(6)	122.9(3)
N(2)-C(6)-C(7)	119.5(3)
N(2)-C(6)-C(5)	114.2(3)
C(7)-C(6)-C(5)	126.3(3)
C(8)-C(7)-C(6)	119.4(3)
C(7)-C(8)-C(9)	119.7(3)
C(7)-C(8)-C(11)	121.2(3)
C(9)-C(8)-C(11)	118.8(3)
C(10)-C(9)-C(8)	119.7(3)
N(2)-C(10)-C(9)	119.1(3)
N(2)-C(10)-C(13)	111.9(3)
C(9)-C(10)-C(13)	128.9(3)
O(2)-C(11)-O(1)	124.3(3)

O(2)-C(11)-C(8)	122.0(3)
O(1)-C(11)-C(8)	113.7(3)
C(13)-C(12)-C(17)	118.0(3)
C(13)-C(12)-Pd	112.9(2)
C(17)-C(12)-Pd	129.1(3)
C(14)-C(13)-C(12)	121.1(3)
C(14)-C(13)-C(10)	123.1(3)
C(12)-C(13)-C(10)	115.8(3)
C(15)-C(14)-C(13)	119.8(4)
C(17)-C(16)-C(15)	121.1(4)
C(16)-C(17)-C(12)	120.5(4)
C(16)-C(15)-C(14)	119.6(4)

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Pd	29(1)	29(1)	29(1)	10(1)	0(1)	5(1)
Cl	44(1)	47(1)	35(1)	18(1)	-1(1)	12(1)
O(1)	44(1)	38(1)	39(2)	14(1)	-6(1)	11(1)
O(2)	54(2)	40(2)	39(2)	-3(1)	-13(1)	17(1)
O(3)	56(2)	56(2)	56(2)	19(2)	-10(2)	12(2)
N(1)	33(2)	34(2)	32(2)	11(1)	1(1)	3(1)
N(2)	29(1)	28(1)	34(2)	10(1)	4(1)	6(1)
C(1)	42(2)	39(2)	31(2)	7(2)	-3(2)	1(2)
C(2)	55(2)	40(2)	34(2)	-1(2)	-3(2)	3(2)
C(3)	56(2)	31(2)	43(2)	0(2)	-1(2)	9(2)
C(4)	44(2)	37(2)	44(2)	10(2)	-1(2)	12(2)
C(5)	29(2)	30(2)	30(2)	9(1)	1(1)	5(1)
C(6)	27(2)	30(2)	28(2)	8(1)	1(1)	4(1)
C(7)	33(2)	28(2)	36(2)	8(2)	3(1)	8(1)
C(8)	28(2)	35(2)	31(2)	12(2)	1(1)	7(1)
C(9)	32(2)	34(2)	28(2)	4(1)	-1(1)	5(1)
C(10)	30(2)	29(2)	31(2)	7(1)	2(1)	4(1)
C(11)	35(2)	42(2)	31(2)	11(2)	6(2)	15(2)
C(12)	28(2)	33(2)	41(2)	14(2)	5(1)	7(1)
C(13)	31(2)	30(2)	37(2)	9(2)	1(1)	6(1)
C(14)	41(2)	34(2)	45(2)	6(2)	-2(2)	7(2)
C(15)	47(2)	30(2)	59(3)	0(2)	-2(2)	10(2)
C(16)	47(2)	30(2)	66(3)	18(2)	5(2)	10(2)
C(17)	38(2)	35(2)	52(2)	19(2)	2(2)	9(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(1B)	12311	3382	9255	61
H(1A)	5888	2526	1872	48
H(2A)	6377	49	1155	58
H(3A)	7874	-792	2544	57
H(4A)	8923	919	4635	51
H(7A)	9936	2742	6610	39
H(9A)	9920	7121	8888	41
H(14A)	8785	9294	8930	51
H(16A)	6467	11215	6772	57
H(17A)	5957	8921	5028	49
H(15A)	7881	11427	8718	60
H(1W)	15050(50)	3500(50)	9800(40)	60
H(2W)	14210(60)	4110(40)	10970(30)	60

Table S6. Torsion angles [deg] for 1.

N(2)-Pd-N(1)-C(1)	-179.6(3)
C(12)-Pd-N(1)-C(1)	-175.7(3)
Cl-Pd-N(1)-C(1)	-1.9(3)
N(2)-Pd-N(1)-C(5)	0.1(2)
C(12)-Pd-N(1)-C(5)	4.0(5)
Cl-Pd-N(1)-C(5)	177.7(2)
C(12)-Pd-N(2)-C(6)	-178.3(3)
N(1)-Pd-N(2)-C(6)	0.4(2)
Cl-Pd-N(2)-C(6)	-114.0(18)
C(12)-Pd-N(2)-C(10)	1.3(2)
N(1)-Pd-N(2)-C(10)	179.9(3)
Cl-Pd-N(2)-C(10)	65.5(19)
C(5)-N(1)-C(1)-C(2)	0.5(5)
Pd-N(1)-C(1)-C(2)	-179.8(3)
N(1)-C(1)-C(2)-C(3)	0.4(6)
C(1)-C(2)-C(3)-C(4)	-0.9(6)
C(2)-C(3)-C(4)-C(5)	0.6(6)
C(1)-N(1)-C(5)-C(4)	-0.9(5)
Pd-N(1)-C(5)-C(4)	179.4(3)
C(1)-N(1)-C(5)-C(6)	179.2(3)
Pd-N(1)-C(5)-C(6)	-0.5(4)
C(3)-C(4)-C(5)-N(1)	0.3(6)
C(3)-C(4)-C(5)-C(6)	-179.7(3)
C(10)-N(2)-C(6)-C(7)	-1.9(5)
Pd-N(2)-C(6)-C(7)	177.7(2)
C(10)-N(2)-C(6)-C(5)	179.7(3)
Pd-N(2)-C(6)-C(5)	-0.7(4)
N(1)-C(5)-C(6)-N(2)	0.8(4)
C(4)-C(5)-C(6)-N(2)	-179.1(3)
N(1)-C(5)-C(6)-C(7)	-177.5(3)
C(4)-C(5)-C(6)-C(7)	2.6(6)
N(2)-C(6)-C(7)-C(8)	0.4(5)
C(5)-C(6)-C(7)-C(8)	178.6(3)
C(6)-C(7)-C(8)-C(9)	0.9(5)
C(6)-C(7)-C(8)-C(11)	-173.4(3)
C(7)-C(8)-C(9)-C(10)	-0.9(5)
C(11)-C(8)-C(9)-C(10)	173.6(3)
C(6)-N(2)-C(10)-C(9)	1.9(5)
Pd-N(2)-C(10)-C(9)	-177.6(2)
C(6)-N(2)-C(10)-C(13)	179.9(3)
Pd-N(2)-C(10)-C(13)	0.3(4)
C(8)-C(9)-C(10)-N(2)	-0.5(5)
C(8)-C(9)-C(10)-C(13)	-178.1(3)
C(7)-C(8)-C(11)-O(2)	158.1(4)
C(9)-C(8)-C(11)-O(2)	-16.3(5)
C(7)-C(8)-C(11)-O(1)	-20.4(5)
C(9)-C(8)-C(11)-O(1)	165.2(3)
N(2)-Pd-C(12)-C(13)	-2.6(2)
N(1)-Pd-C(12)-C(13)	-6.5(5)
Cl-Pd-C(12)-C(13)	179.7(2)
N(2)-Pd-C(12)-C(17)	177.2(3)
N(1)-Pd-C(12)-C(17)	173.3(3)
Cl-Pd-C(12)-C(17)	-0.5(3)
C(17)-C(12)-C(13)-C(14)	1.6(5)
Pd-C(12)-C(13)-C(14)	-178.6(3)
C(17)-C(12)-C(13)-C(10)	-176.2(3)
Pd-C(12)-C(13)-C(10)	3.6(4)
N(2)-C(10)-C(13)-C(14)	179.7(3)
C(9)-C(10)-C(13)-C(14)	-2.6(6)

N(2)-C(10)-C(13)-C(12)	-2.6(4)
C(9)-C(10)-C(13)-C(12)	175.1(3)
C(12)-C(13)-C(14)-C(15)	-1.9(6)
C(10)-C(13)-C(14)-C(15)	175.7(4)
C(15)-C(16)-C(17)-C(12)	-0.2(6)
C(13)-C(12)-C(17)-C(16)	-0.5(5)
Pd-C(12)-C(17)-C(16)	179.7(3)
C(17)-C(16)-C(15)-C(14)	-0.1(6)
C(13)-C(14)-C(15)-C(16)	1.1(6)

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z

Table S7. Hydrogen bonds for 1 [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1B)...O(3)#1	0.82	1.76	2.581(4)	175.8
O(3)-H(1W)...O(2)#2	0.94(3)	2.15(4)	2.918(4)	138(4)
O(3)-H(2W)...Cl#3	0.95(3)	2.26(3)	3.176(4)	161(4)

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z #2 -x+3,-y+1,-z+2 #3 x+1,y,z+1