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Characterization of a Pd^{II} complex with (*E*)-8-hydroxyquinoline-2-carbaldehyde *O*-benzyl oxime

Jan G. Małecki, Anna Maroń, Izabela Gryca and Maciej Serda

Tables:

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Table S1 Crystal data and structures refinement details of (*E*)-8-hydroxyquinoline-2-carbaldehyde *O*-benzyl oxime (**L**) and [Pd(L)$_2$] complex.

Empirical formula	$C_{17}H_{14}N_2O_2$	$C_{34}H_{26}N_4O_4Pd$
Formula weight	278.30	660.99
Temperature [K]	295.0(2) K	295.0(2) K
Crystal system	monoclinic	triclinic
Space group	$P2_1/c$	P-1
Unit cell dimensions		
a [Å]	13.7263(13)	4.8859(3)
b [Å]	11.3149(11)	9.0453(5)
c [Å]	9.1935(9)	16.0294(11)
α	90	89.011(5)
β	103.803(9)	87.620(6)
γ	90	83.387(5)
Volume [Å^3]	1386.6(2)	703.04(8)
Z	4	1
Calculated density [Mg/m^3]	1.333	1.561
Absorption coefficient [mm^{-1}]	0.089	0.708
F(000)	584	336
Crystal dimensions [mm]	0.47 x 0.21 x 0.11	0.44 x 0.05 x 0.02
θ range for data collection [º]	3.60 to 25.05	3.39 to 25.05
Index ranges	-16<=h<=14	-5<=h<=5
	-13<=k<=13	-10<=k<=10
	-10<=l<=10	-19<=l<=18
Reflections collected	6585	4545
Independent reflections	2447 [$R_{(int)}$ = 0.0282]	2181 [$R_{(int)}$ = 0.0577]
Data / restraints / parameters	2447/0/191	2480/0/232
Goodness-of-fit on F^2	0.998	1.049
Final R indices [I>2σ(I)]	R_1 = 0.0446	R_1 = 0.0580
	wR_2 = 0.0966	wR_2 = 0.1291
R indices (all data)	R_1 = 0.0731	R_1 = 0.0620
	wR_2 = 0.1070	wR_2 = 0.1315
Largest diff. peak and hole	0.132 and -0.214	1.503 and -1.202

Table S2 Selected bond lengths [Å] and angles [º] for (*E*)-8-hydroxyquinoline-2-carbaldehyde *O*-benzyl oxime (**L**) and [Pd(L)$_2$] complex.

bond lengths [Å]	exp	calc
(**L**)		
O(1)-C(8)	1.3484(19)	
O(2)-N(2)	1.3990(16)	
O(2)-C(11)	1.4431(18)	
N(1)-C(1)	1.3260(18)	
N(1)-C(9)	1.3630(18)	
N(2)-C(10)	1.2666(18)	
[Pd(L)$_2$]		
Pd(1)-O(1)	1.986(3)	2.033
Pd(1)-N(1)	2.076(4)	2.154
O(1)-C(8)	1.307(6)	1.315
O(2)-N(2)	1.389(5)	1.383
O(2)-C(11)	1.430(7)	1.44
N(1)-C(1)	1.341(6)	1.337
N(1)-C(9)	1.380(6)	1.379
N(2)-C(10)	1.261(7)	1.281
angles [º]		
(**L**)		
(N2)-O(2)-C(11)	108.80(12)	
C(1)-N(1)-C(9)	117.15(14)	
C(1)-N(2)-O(2)	110.96(13)	
N(1)-C(1)-C(2)	122.91(14)	
N(1)-C(1)-C(10)	115.63(14)	
O(1)-C(8)-C(7)	120.42(14)	
N(1)-C(9)-C(4)	124.00(14)	
N(1)-C(9)-C(8)	116.72(14)	
N(2)-C(10)-C(1)	120.07(15)	
O(2)-C(11)-C(12)	112.38(13)	
[Pd(L)$_2$]		
O(1)-Pd(1)-N(1)	81.95(14)	80.29
N(1)-C(1)-C(2)	120.6(4)	120.9
N(1)-C(1)-C(10)	119.1(4)	119.4
N(1)-C(9)-C(4)	123.5(4)	122.6
N(1)-C(1)-C(10)	115.8(4)	117.0

Table S3 Hydrogen bonds for L and [Pd(L)$_2$] complex (Å and º).

D-H···A	d(D–H)	d(H···A)	d(D···A)	<(DHA)
(**L**)				
O(1)–H(1)...N(1)	0.82	2.24	2.7001(16)	115.7
O(1)–H(1)...O(2) #1	0.82	2.42	2.9452(15)	122.7
(**[Pd(L)$_2$]**)				
C(10)–H(10)...O(1) #2	0.93	1.99	2.834(7)	149.5

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

Table S4 π-stacking interaction in structure of (*E*)-8-hydroxyquinoline-2-carbaldehyde *O*-benzyl oxime

Centroids: #Cg1: (C4-C9); #Cg2: (N1;C9;C4;C3;C2;C1)			
	angle [º]	distance [Å]	shift angle [Å]
#Cg1: #Cg2 [*x,1/2-y,1/2+z*]	4.833	3.671	1.133

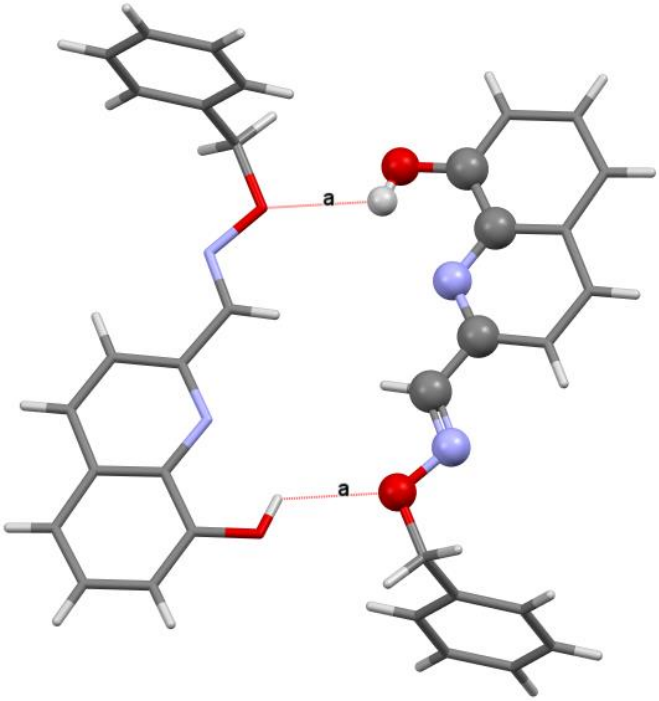

Figure S1 Dimer of $R_2^2(18)$ type in molecular structure of (*E*)-8-hydroxyquinoline-2-carbaldehyde *O*-benzyl oxime.

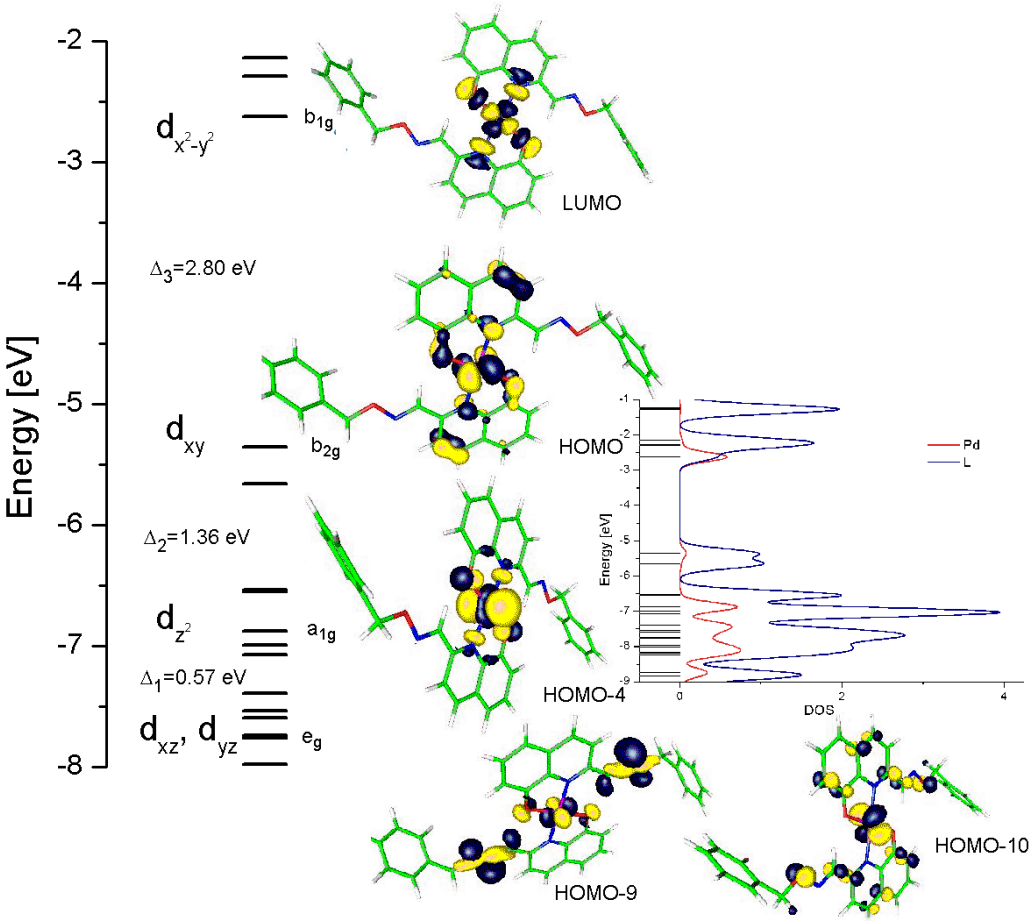

Figure S2 Splitting of 4*d* palladium(II) orbital diagram for the complex.