Palladium(II)- and Platinum(II)phenyl-2,6-bis(oxazole) pincer complexes. Syntheses, crystal structures, and photophysical properties.

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Supporting Information

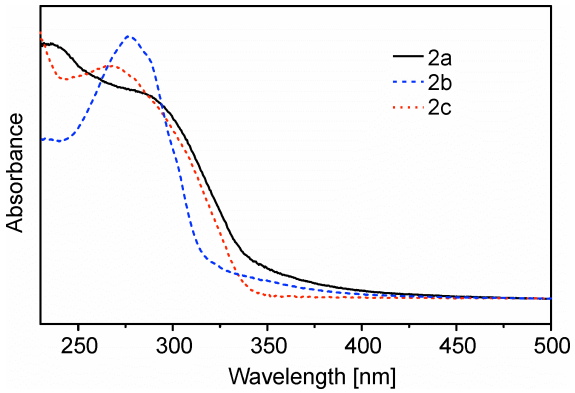


Fig. S1. Absorption spectra of the ligands **2a-2c** at ambient temperature in CH_2Cl_2.

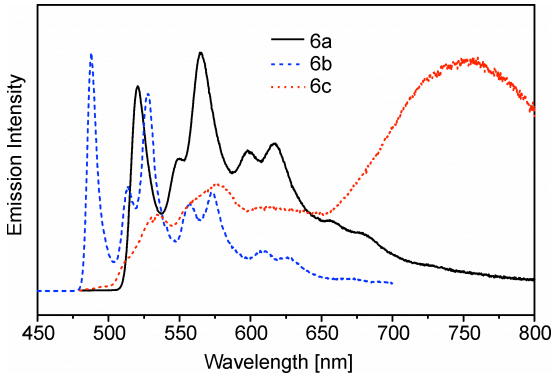


Fig. S3. Emission spectra of the Pd(II) compounds **6a-6c** at 77 K in ethanol.

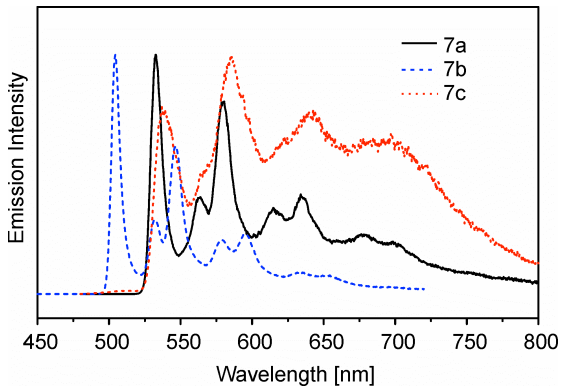
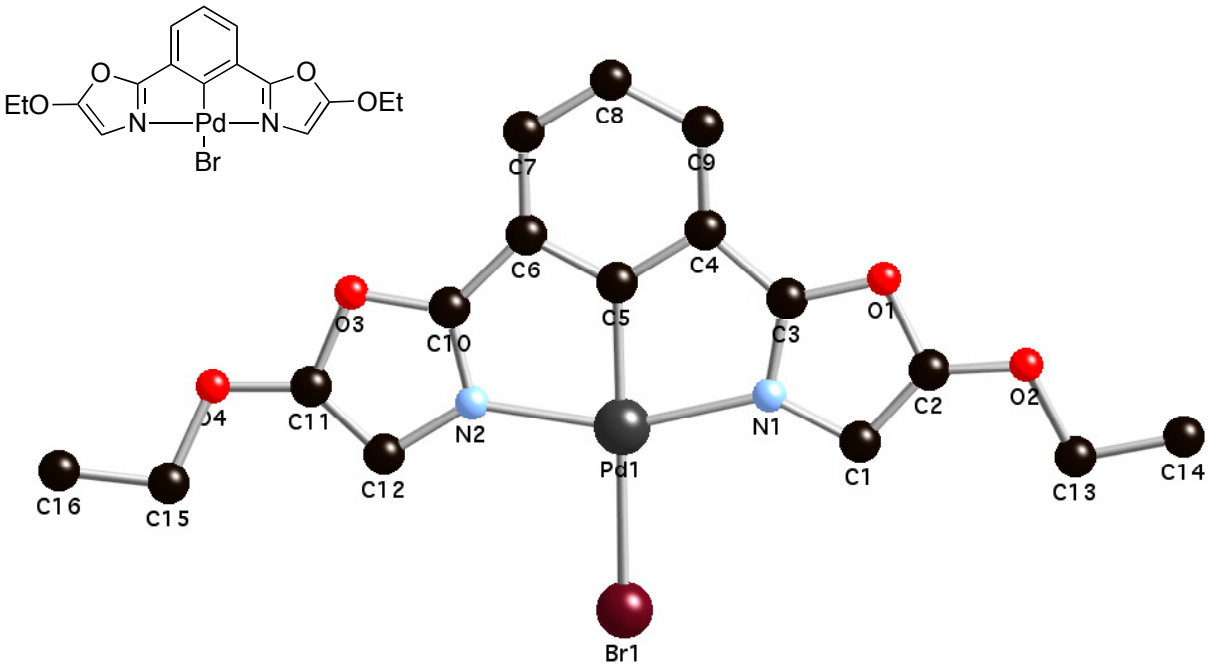


Fig. S3. Emission spectra of the Pt(II) compounds **7a-7c** at 77 K in ethanol.

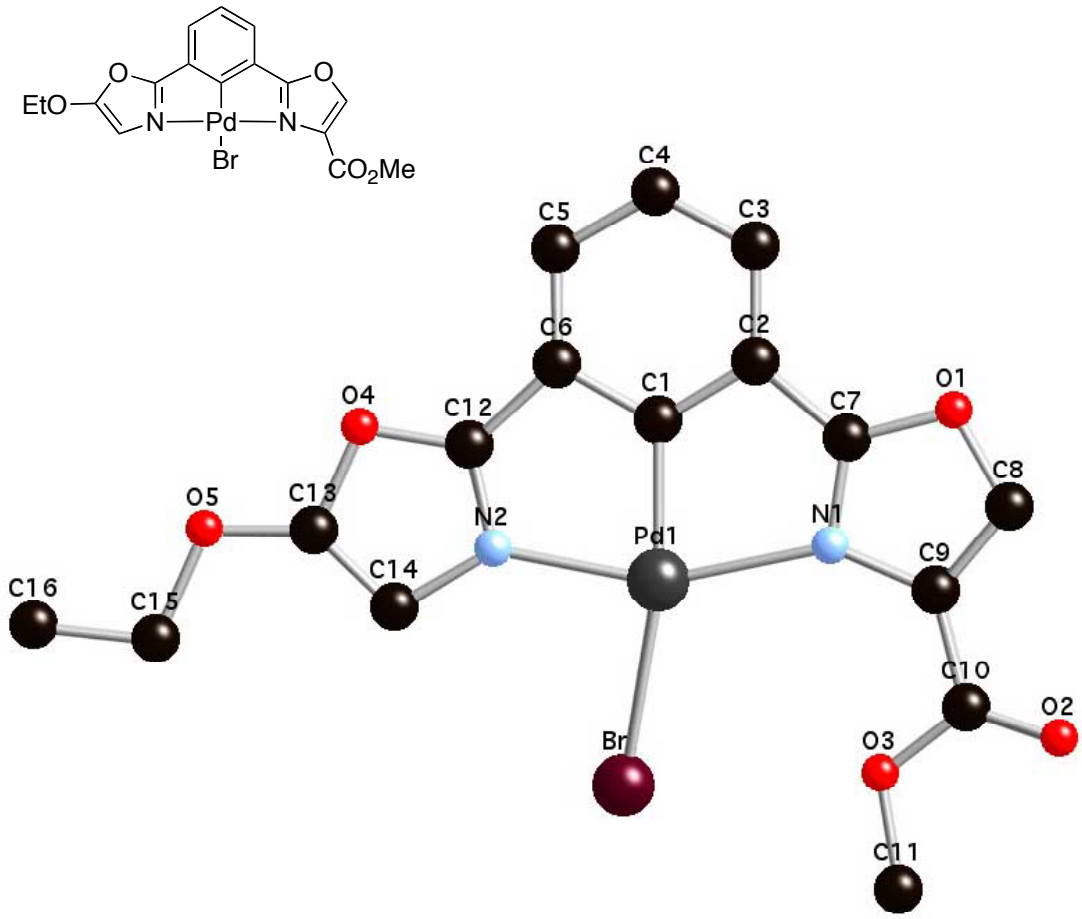
Table 1. Crystal data and structure refinements for compounds **6a, 6c, 7a** and **7c**.

Compound	**6a**	**6c**	**7a**	**7b**
Empirical formula	$C_{16}H_{15}BrN_2O_4Pd$	$C_{16}H_{13}BrN_2O_5Pd$	$C_{16}H_{15}BrN_2O_4Pt$	$C_{16}H_{13}BrN_2O_5Pt$
Formula weight	485.62	499.60	574.28	588.26
Crystal size (mm)	0.32 x 0.20 x 0.08	0.30 x 0.26 x 0.14	0.48 x 0.12 x 0.02	0.49 x 0.21 x 0.12
Crystal description	prism	prism	rod	prism
Crystal colour	light yellow	yellow to orange	light yellow	yellow to orange
Crystal system	monoclinic	triclinic	monoclinic	triclinic
Space group	$P2_1/c$	P-1	$C2/c$	P-1
a (Å)	7.5601(8)	9.6564(11)	33.697(4)	9.6961(10)
b (Å)	9.3101(6)	10.0610(12)	5.2354(4)	10.0725(10)
c (Å)	24.686(3)	10.5897(12)	19.994(2)	10.4364(10)
α (°)		107.986(13)		107.818(11)
β (°)	90.828(12)	112.136(12)	96.702(14)	111.729(11)
γ (°)		100.062(13)		99.999(12)
Volume (Å³)	1737.4(3)	855.5(2)	3503.2(6)	852.7(2)
Z	4	2	8	2
d(calc.) (Mg/m³)	1.857	1.939	2.178	2.291
μ (mm^{-1})	3.390	3.449	10.313	10.600
F(000)	952	488	2160	552
Measurement device type	STOE-IPDS	STOE-IPDS	STOE-IPDS	STOE-IPDS
Measurement method	rotation	rotation	rotation	rotation
Temperature (K)	173(1)	173(1)	173(1)	173(1)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
monochromator	graphite	graphite	graphite	graphite
Θ range (°)	3.18, 25.87	2.41, 27.93	2.26, 25.87	2.25, 26.85
Refl. collected/unique	19590 / 3360	10880 / 3756	6524 / 1688	10760 / 3422
R(int)	0.0360	0.0326	0.0834	0.0339
Reflections I>2σ(I)	2905	3258	1450	3092
Absorption correction	analytical	analytical	numerical	numerical
Max./min. transmission	0.7642 / 0.4459	0.7039 / 0.3711	0.2564/ 0.1554	0.3258/ 0.0539
Data/ parameters	3360 / 217	3756 / 226	1688 / 217	3422 / 226
Goodness-of-fit on F^2	0.969	0.963	1.021	1.029
R_1, wR_2 [I>2σ(I)]	0.0226, 0.0560	0.0238, 0.0580	0.0461, 0.1225	0.0233, 0.0563
R_1, wR_2 (all data)	0.0272, 0.0571	0.0293, 0.0596	0.0513, 0.1272	0.0265, 0.0572
Residual density ($eÅ^{-3}$)	0.680/-0.290	0.466/ -0.376	1.792/ -1.567	0.676/ -1.521

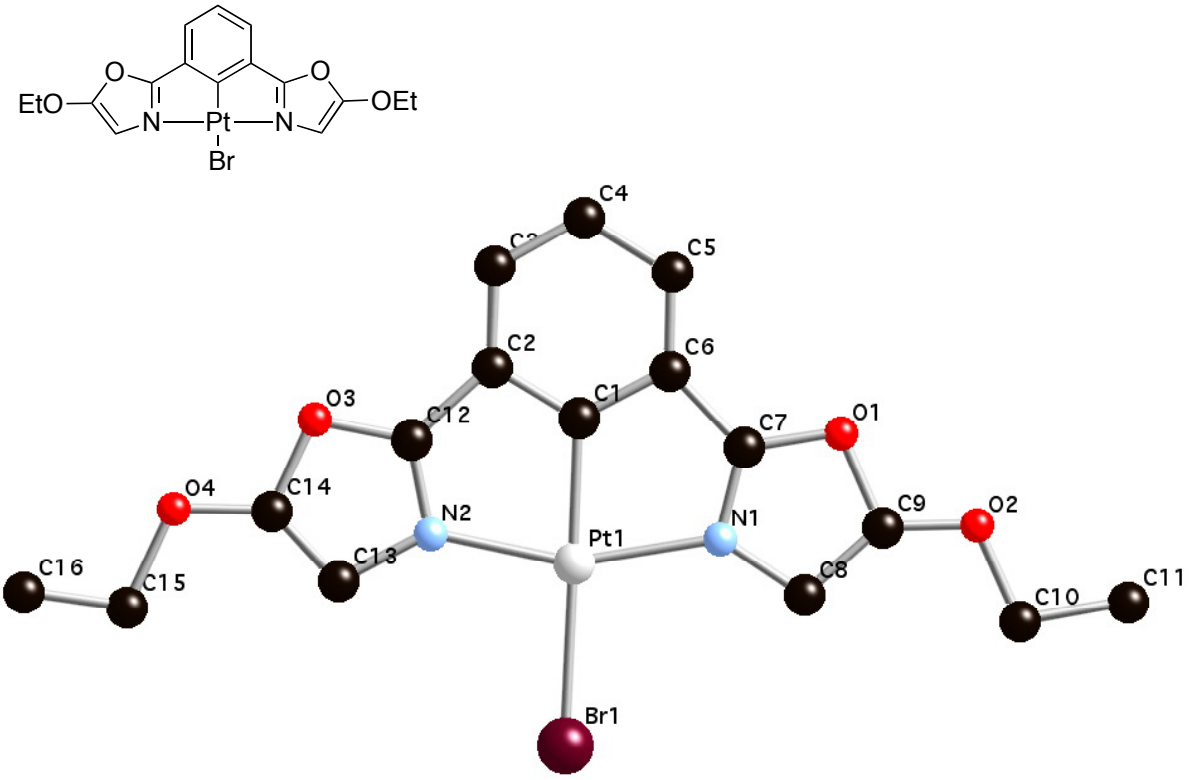
6a



6c



7a



7c