Non-covalent stacking interactions directing the structural and photophysical features of mono- and dinuclear cyclometallated palladium(II) complexes

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Electronic Supplementary Information

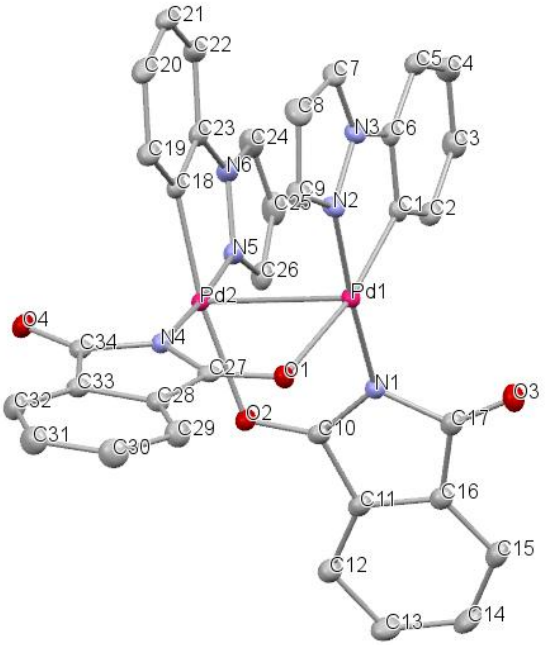

Figure S1. ORTEP plot of complex **I3**

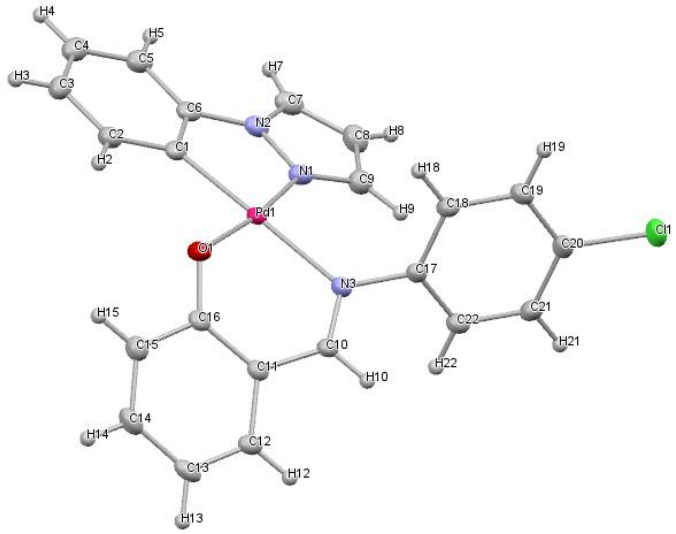

Figure S2. ORTEP plot of complex **I5**

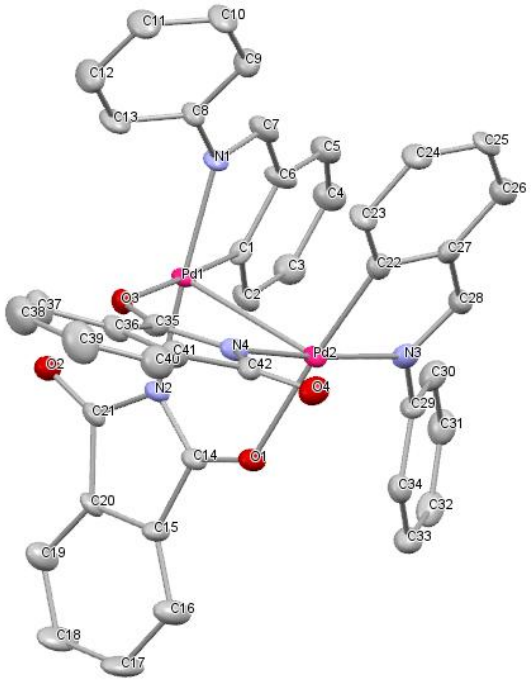

Figure S3. ORTEP plot of complex **II3**

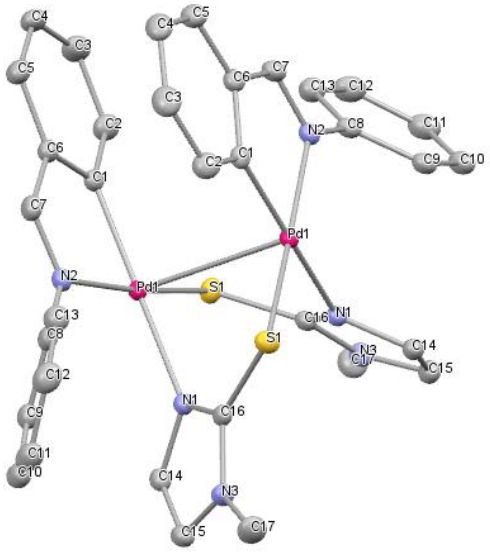

Figure S4. ORTEP plot of complex **II4**

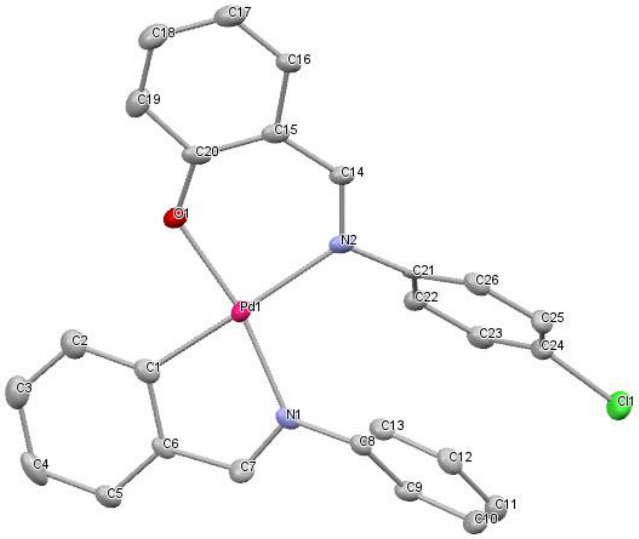

Figure S5. ORTEP plot of complex **II5**

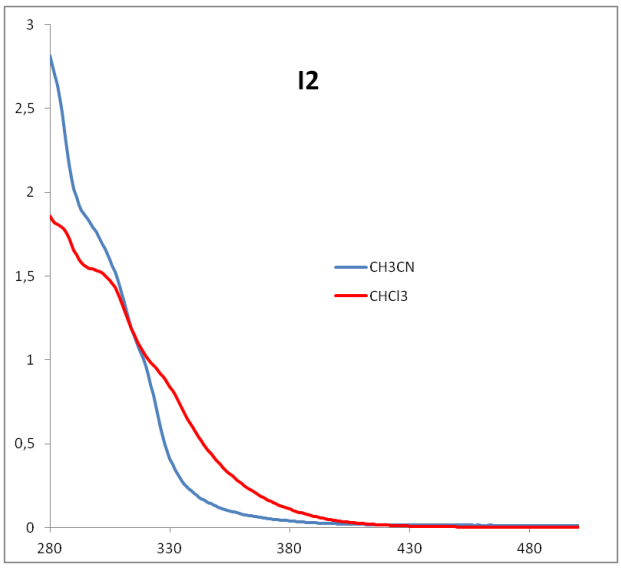

Figure S6. Absorption spectra of complex **I2** in chloroform and acetonitrile solutions.

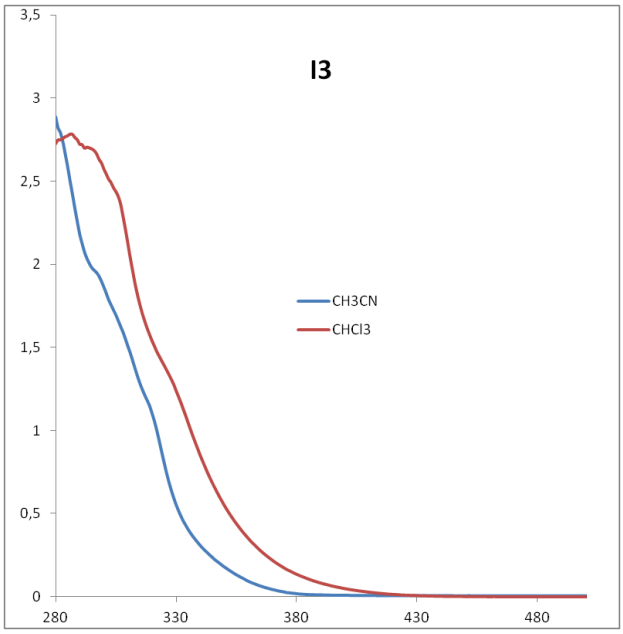

Figure S7. Absorption spectra of complex **I3** in chloroform and acetonitrile solutions.

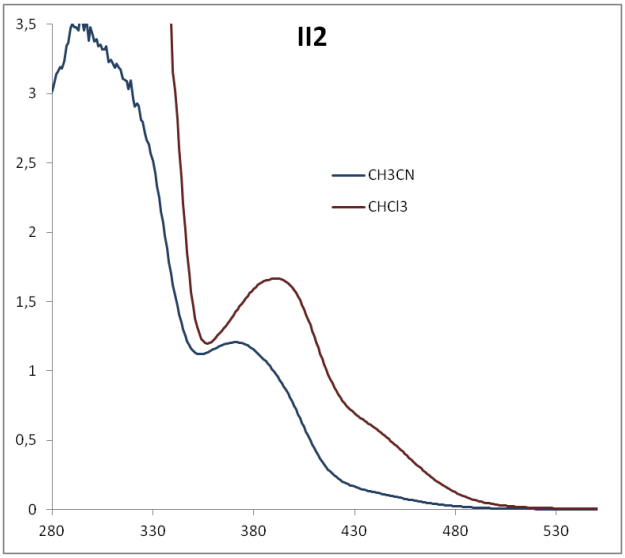

Figure S8. Absorption spectra of complex **II2** in chloroform and acetonitrile solutions.

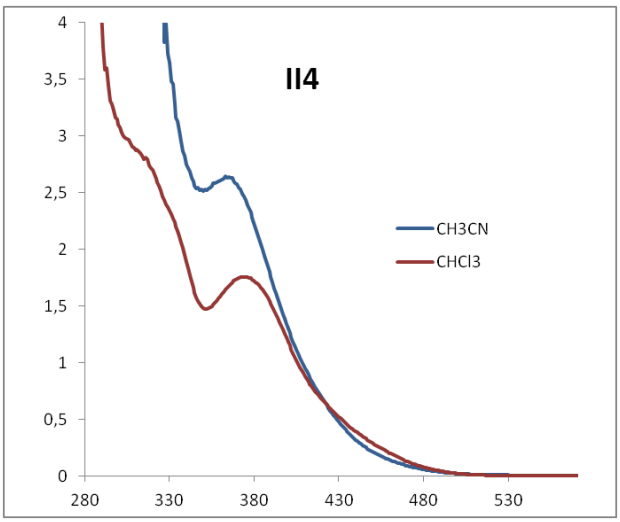

Figure S9. Absorption spectra of complex **II4** in chloroform and acetonitrile solutions.

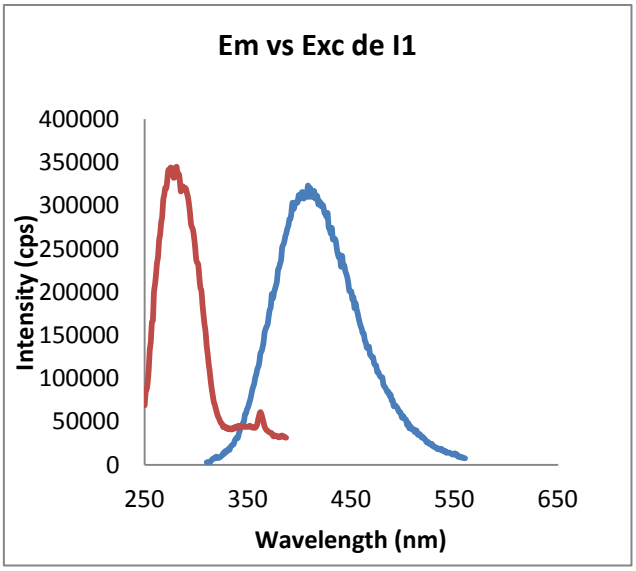

Figure S10. Emission (blue line) and excitation (red line) spectra of complex **I1** in chloroform solution.

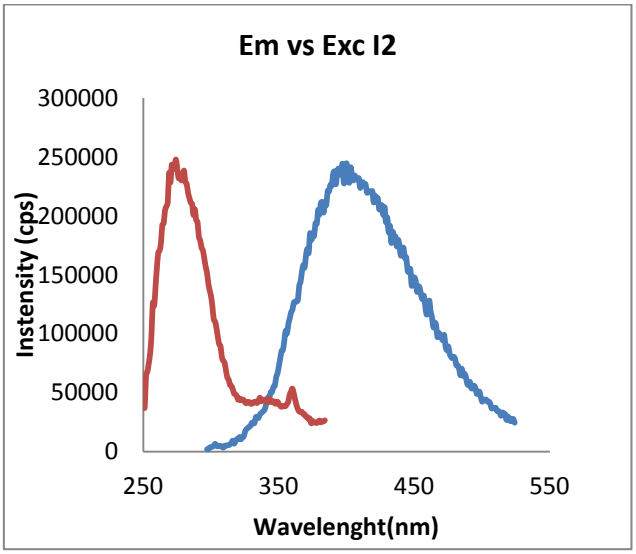

Figure S11. Emission (blue line) and excitation (red line) spectra of complex **I2** in chloroform solution.

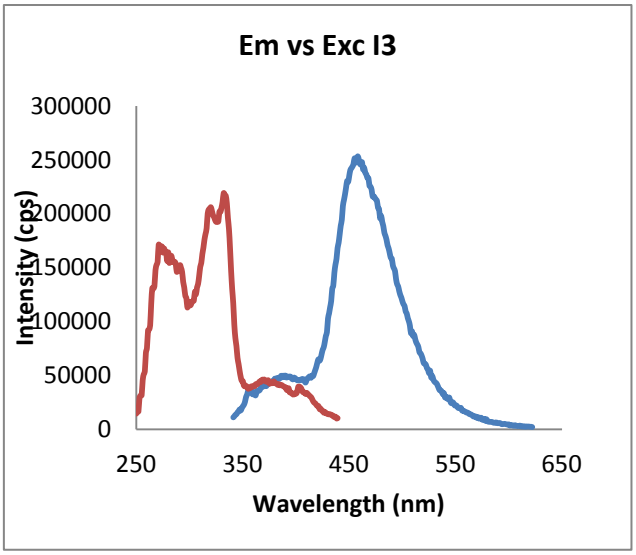

Figure S12. Emission (blue line) and excitation (red line) spectra of complex **I3** in chloroform solution.

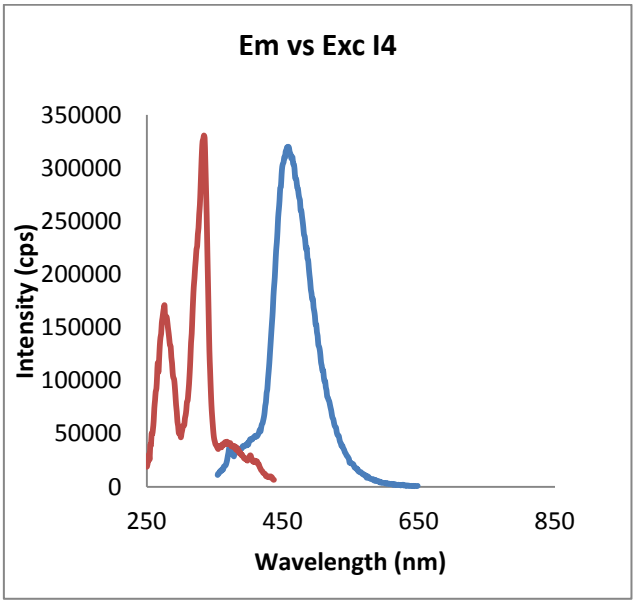

Figure S13. Emission (blue line) and excitation (red line) spectra of complex **I4** in chloroform solution.

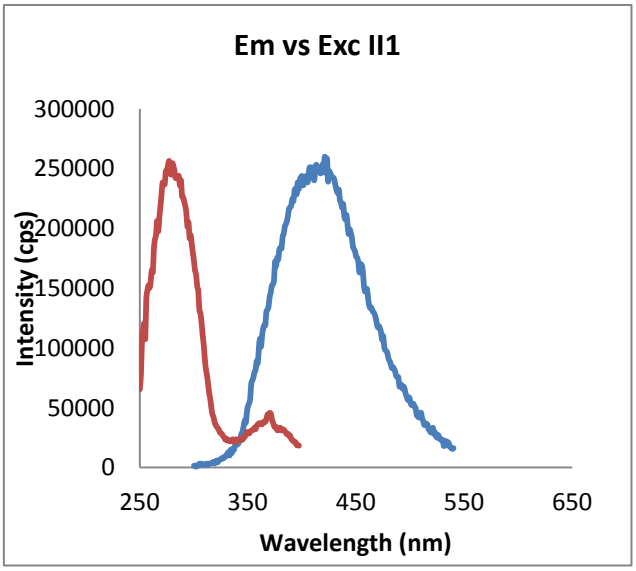

Figure S14. Emission (blue line) and excitation (red line) spectra of complex **II1** in chloroform solution.

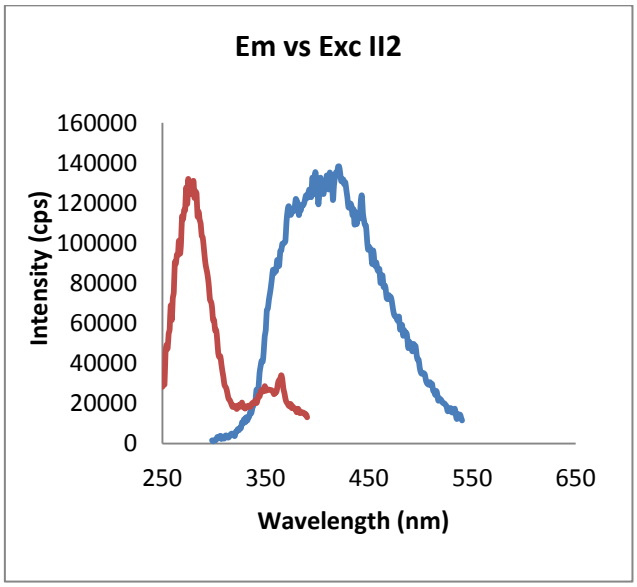

Figure S15. Emission (blue line) and excitation (red line) spectra of complex **II2** in chloroform solution.

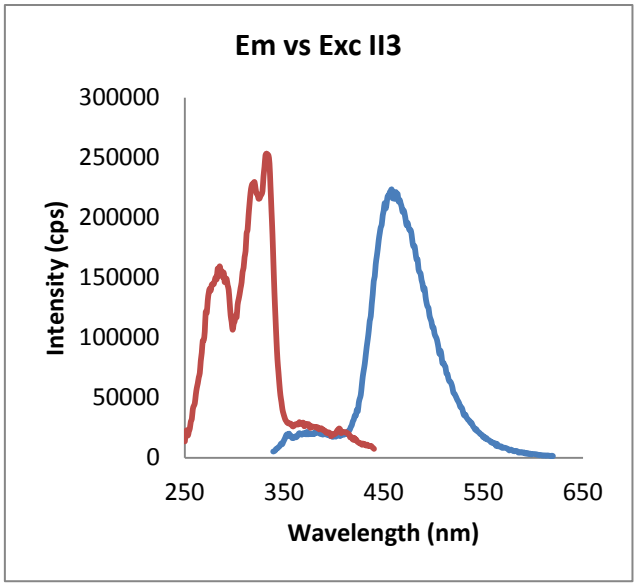

Figure S16. Emission (blue line) and excitation (red line) spectra of complex **II3** in chloroform solution.

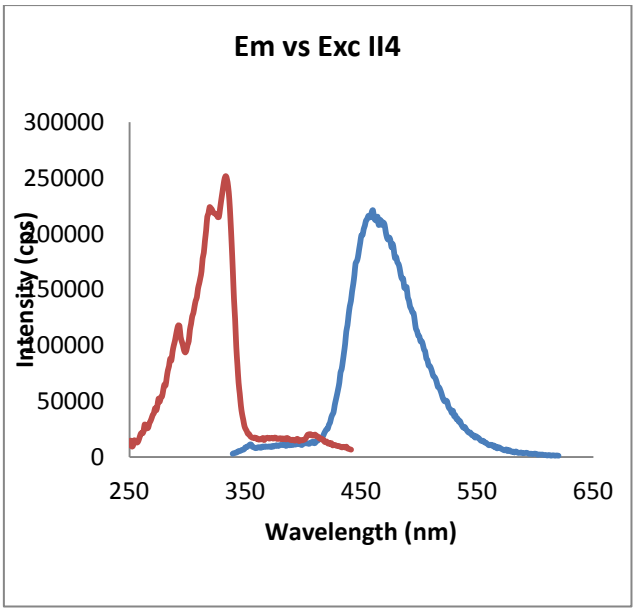

Figure S17. Emission (blue line) and excitation (red line) spectra of complex **II4** in chloroform solution.

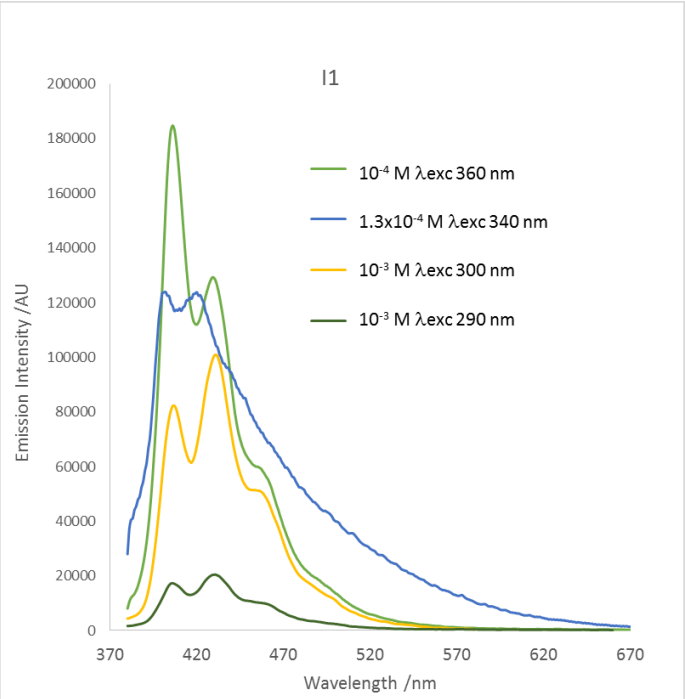

Figure S18. Emission spectrum of complex **I1** at different concentrations in chloroform solutions.

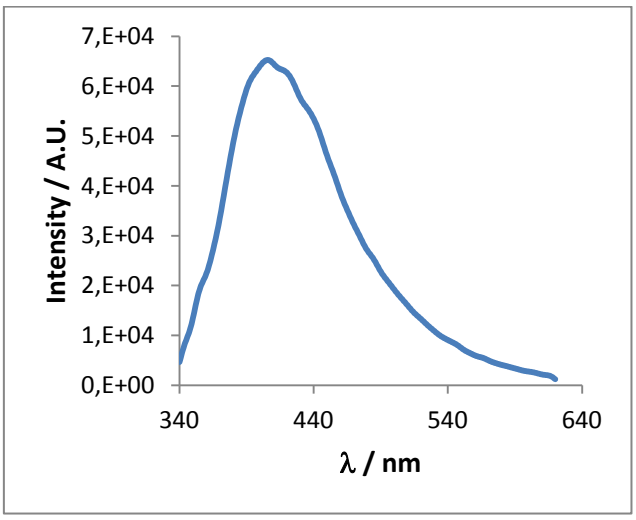

Figure S19. Emission spectrum of complex **I2** in chloroform solution at 1.7 x 10^{-4} M λ_{exc} 320 nm.

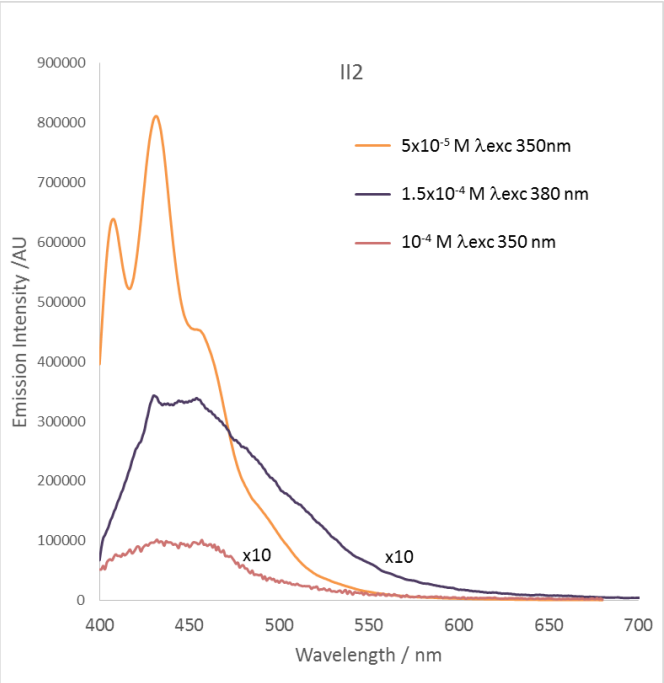

Figure S20. Emission spectrum of complex **II2** at different concentrations in chloroform solutions.

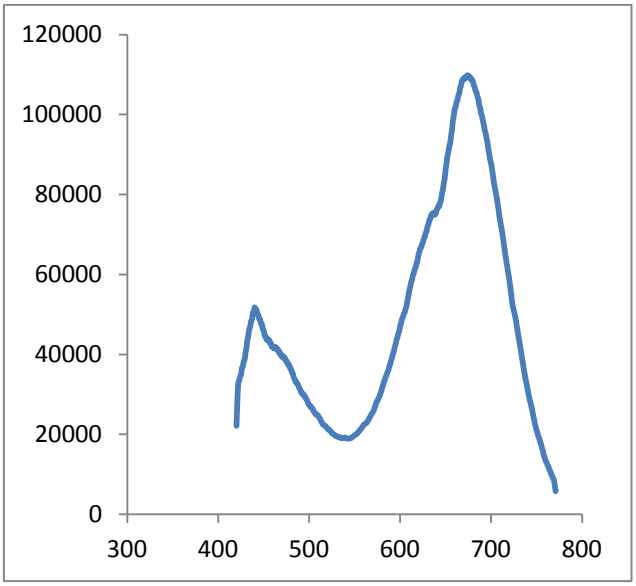

Figure S21. Emission spectra of complex **I2** in solid state

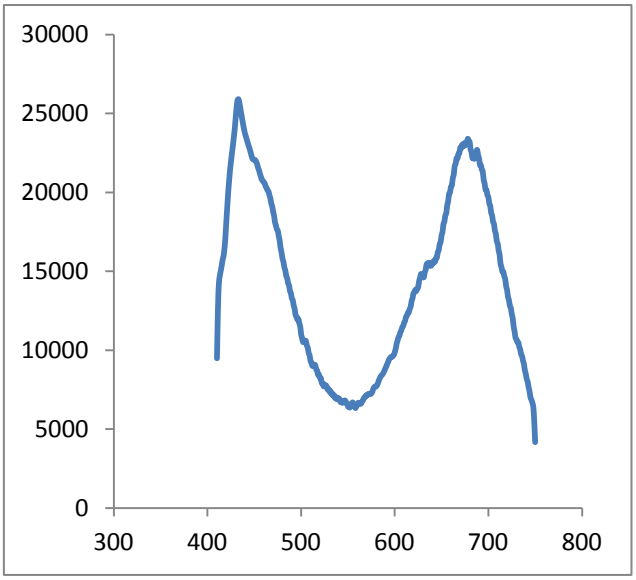

Figure S22. Emission spectra of complex **I3** in solid state

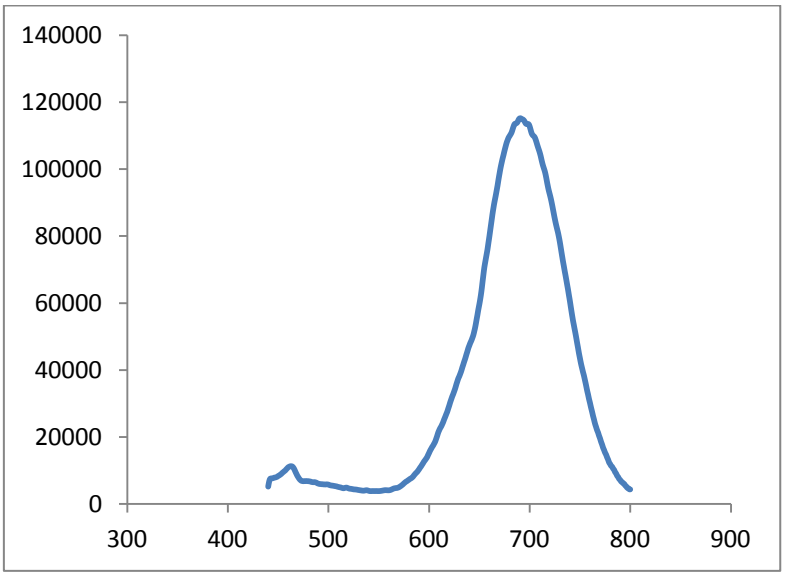

Figure S23. Emission spectra of complex **I1** in solid state

Table S1

Calculated density		
	Series I	Series II
Ligand 1	1.854	1.704
Ligand 4	1.835	1.728
Ligand 5	1.704	1.613

Table S2. Crystal data and structure refinement for **I3**

Identification code	I3	
Empirical formula	$C_{38}H_{32}N_6O_5Pd_2$	
Formula weight	865.50	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.7725(6) Å	α= 70.7900(10)°
	b = 12.4247(9) Å	β= 84.1970(10)°
	c = 16.5407(12) Å	γ = 87.9410(10)°
Volume	1693.7(2) $Å^3$	
Z	2	
Density (calculated)	1.697 Mg/m^3	
Absorption coefficient	1.117 mm^{-1}	
F(000)	868	
Crystal size	0.31 x 0.15 x 0.14 mm^3	
Theta range for data collection	1.31 to 28.59°	
Index ranges	-11<=h<=11, -16<=k<=16, -22<=l<=22	
Reflections collected	20743	
Independent reflections	7942 [R(int) = 0.0162]	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7942 / 0 / 460	
Goodness-of-fit on F^2	1.179	
Final R indices [I>2sigma(I)]	R1 = 0.0222, wR2 = 0.0572	
R indices (all data)	R1 = 0.0238, wR2 = 0.0639	
Largest diff. peak and hole	0.632 and -0.607 $e.Å^{-3}$	

Table S3. Crystal data and structure refinement for **I5**

Identification code	I5	
Empirical formula	$C_{22}H_{16}ClN_3OPd$	
Formula weight	480.23	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.3070(6) Å	α= 93.918(2)°
	b = 10.4711(7) Å	β= 102.381(2)°
	c = 10.4887(7) Å	γ = 108.576(2)°
Volume	936.02(11) $Å^3$	
Z	2	
Density (calculated)	1.704 Mg/m^3	
Absorption coefficient	1.152 mm^{-1}	
F(000)	480	
Crystal size	0.17 x 0.09 x 0.05 mm^3	
Theta range for data collection	2.01 to 29.45°	
Index ranges	-12<=h<=12, -14<=k<=14, -14<=l<=14	
Reflections collected	29136	
Independent reflections	5189 [R(int) = 0.0393]	
Absorption correction	None	
Max. and min. transmission	0.9446 and 0.8282	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5189 / 0 / 253	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0313, wR2 = 0.0767	
R indices (all data)	R1 = 0.0383, wR2 = 0.0799	
Largest diff. peak and hole	1.194 and -1.266 $e.Å^{-3}$	

Table S4. Crystal data and structure refinement for **II3**

Identification code	II3	
Empirical formula	$C_{43}H_{30}Cl_2N_4O_4Pd_2$	
Formula weight	950.41	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 9.7804(10) Å	α= 90°
	b = 17.4573(18) Å	β= 97.068(3)°
	c = 22.148(2) Å	γ = 90°
Volume	3752.7(7) $Å^3$	
Z	4	
Density (calculated)	1.682 Mg/m^3	
Absorption coefficient	1.151 mm^{-1}	
F(000)	1896	
Crystal size	0.18 x 0.03 x 0.03 mm^3	
Theta range for data collection	2.10 to 29.95°	
Index ranges	-13<=h<=12, -24<=k<=24, -29<=l<=31	
Reflections collected	54211	
Independent reflections	10701 [R(int) = 0.1224]	
Absorption correction	None	
Max. and min. transmission	0.9663 and 0.8196	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10701 / 0 / 481	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0763, wR2 = 0.1244	
R indices (all data)	R1 = 0.1786, wR2 = 0.1602	
Largest diff. peak and hole	1.761 and -2.490 $e.Å^{-3}$	

Table S5. Crystal data and structure refinement for **II4**

Identification code	II4	
Empirical formula	$C_{34}H_{30}N_6Pd_2S_2$	
Formula weight	799.56	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 23.5263(19) Å	α= 90°
	b = 10.5734(8) Å	β= 116.96°
	c = 13.8590(11) Å	γ = 90°
Volume	3072.9(4) $Å^3$	
Z	4	
Density (calculated)	1.728 Mg/m^3	
Absorption coefficient	1.342 mm^{-1}	
F(000)	1600	
Crystal size	0.31 x 0.18 x 0.10 mm^3	
Theta range for data collection	1.94 to 28.65°	
Index ranges	-31<=h<=31, -13<=k<=14, -18<=l<=18	
Reflections collected	18269	
Independent reflections	3749 [R(int) = 0.0178]	
Absorption correction	None	
Max. and min. transmission	0.8775 and 0.6810	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3749 / 0 / 211	
Goodness-of-fit on F^2	1.100	
Final R indices [I>2sigma(I)]	R1 = 0.0201, wR2 = 0.0506	
R indices (all data)	R1 = 0.0208, wR2 = 0.0511	
Largest diff. peak and hole	0.378 and -0.578 $e.Å^{-3}$	

Table S6. Crystal data and structure refinement for **II5**

Identification code	II5	
Empirical formula	$C_{26}H_{19}ClN_2OPd$	
Formula weight	517.28	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	P212121	
Unit cell dimensions	a = 9.3779(8) Å	α= 90°
	b = 10.1838(9) Å	β= 90°
	c = 22.3045(18) Å	γ = 90°
Volume	2130.1(3) $Å^3$	
Z	4	
Density (calculated)	1.613 Mg/m^3	
Absorption coefficient	1.018 mm^{-1}	
F(000)	1040	
Crystal size	0.26 x 0.11 x 0.05 mm^3	
Theta range for data collection	2.20 to 31.07°	
Index ranges	-13<=h<=13, -14<=k<=14, -31<=l<=29	
Reflections collected	31348	
Independent reflections	6520 [R(int) = 0.1003]	
Absorption correction	None	
Max. and min. transmission	0.9509 and 0.7778	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6520 / 0 / 280	
Goodness-of-fit on F^2	1.003	
Final R indices [I>2sigma(I)]	R1 = 0.0475, wR2 = 0.0949	
R indices (all data)	R1 = 0.0726, wR2 = 0.1002	
Absolute structure parameter	0.97(3)	
Largest diff. peak and hole	2.770 and -1.646 $e.Å^{-3}$	