

Electronic Supplementary Information

Phosphorescent platinum(II) complexes containing different β -diketonate ligands: synthesis, tunable excited-state properties, and their application in bioimaging

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Fig. S8 Viability of KB cells with **5** (from left to right: 0, 3, 6.25, 12.5, 25, 50, 100 μ M).

Table S1 Crystallographic data for **4**

Compound reference	Pt(ppy)(DBM) (4)
Chemical formula	C ₂₆ H ₁₉ NO ₂ Pt
Formula Mass	572.51
Crystal system	Monoclinic
<i>a</i> /Å	13.9545(14)
<i>b</i> /Å	7.8076(8)
<i>c</i> /Å	19.5196(19)
α /°	90.00
β /°	109.6850(10)
γ /°	90.00
Unit cell volume/Å ³	2002.4(3)
Temperature/K	291(2)
Space group	<i>P</i> 21/ <i>c</i>
No. of formula units per unit cell, <i>Z</i>	4
Radiation type	MoK α
Absorption coefficient, μ /mm ⁻¹	7.031
No. of reflections measured	9610
No. of independent reflections	3503
<i>R</i> _{int}	0.1354
Final <i>R</i> _{<i>I</i>} values (<i>I</i> > 2 σ (<i>I</i>))	0.0435
Final <i>wR</i> (<i>F</i> ²) values (<i>I</i> > 2 σ (<i>I</i>))	0.1018
Final <i>R</i> _{<i>I</i>} values (all data)	0.0520
Final <i>wR</i> (<i>F</i> ²) values (all data)	0.1130
Goodness of fit on <i>F</i> ²	1.017
CCDC number	758055

Table S2 Coordination bonding parameters (Å, deg) observed in the Pt(II) complexes

complex	Pt-C	Pt-N	Pt-O	C-Pt-N	C-Pt-O	N-Pt-O	O-Pt-O
4	1.963(7)	1.978(7)	2.081(5)	81.2(3)	174.5(2)	93.5(2)	90.71(19)
			2.014(5)		94.6(2)	175.8(2)	
Pt(ppy) ₂ ¹	1.984(4)	2.125(3)		112.8(2)			
Pt(ppy-3-NO ₂)(acac) ²	1.965(4)	1.990(3)	2.089(3)	81.6(16)	175.1(14)	93.6(13)	92.16(12)
			1.998(3)		92.65(15)	174.16(13)	
Pt(ppy-4-tyryl-OMe)(acac) ³	1.970(4)	1.984(3)	2.089(3)	81.6(17)	174.7(15)	93.11(4)	91.60(13)
			2.000(3)		93.69(16)	175.28(13)	

References

- (1) C. M. Laurent, Y. Z. Edgar, Alexander, *Inorg. Chem.*, 1984, **23**, 4249.
- (2) M. D. Perez, P. I. Djurovich, A. Hassan, G. Y. Cheng, T. J. Stewart, K. Aznavour R., Bau and M. E. Thompson, *Chem. Commun.*, 2009, 4215.
- (3) B. L. Yin, F. Niemeyer, J. A. Williams, J. Jiang, A. Boucekkinne, L. Toupet, B. H. Le and V. Guerchais, *Inorg. Chem.*, 2006, **45**, 8584.

Table S3 HOMOs and LUMOs distributions of **1-5** at the lowest singlet state

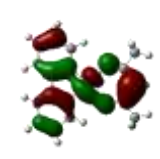
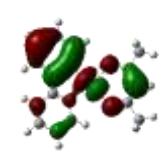
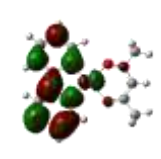
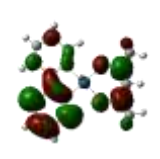
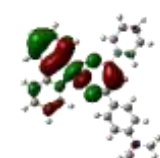
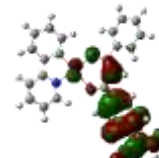
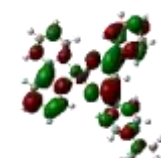
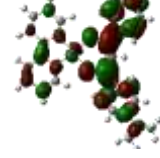
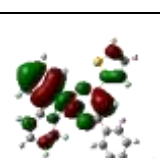
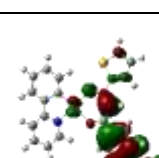
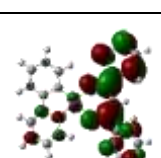
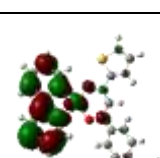

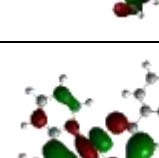
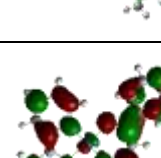
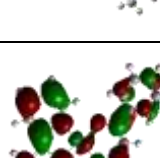
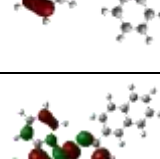
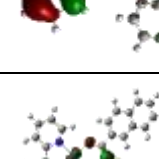
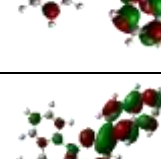
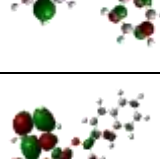
complexes	HOMO-1	HOMO	LUMO	LUMO+1
1				
2				
3				
4				
5				

Table S4 The singlet-state and triplet-state energy levels of different β -diketonate ligands

ligands	Hacac	HNDBM	HNPTPD	HDBM	HCPNPD
T_1/cm^{-1}	22200	18520	not measured	19610	not measured
S_1/cm^{-1}	32895	22272	21692	26042	22936

Table S5 Absorption of **1-5** in CH_2Cl_2 solution from TDDFT Calculations

complex	states	λ (nm)	E (eV)	oscillator	main configurations (CI coeff)	assignment
1	S1	379	3.26	0.0555	HOMO→LUMO (0.65)	LC/MLCT
	S3	341	3.64	0.0839	HOMO-1→LUMO (0.63)	LC/MLCT/LLCT
2	S1	399	3.10	0.4322	HOMO→LUMO (0.66)	MLCT/LLCT/ILCT
	S2	389	3.18	0.2255	HOMO→LUMO+1 (0.50)	MLCT/ILCT/LLCT
3	S1	418.34	2.9637	0.5897	HOMO→LUMO (0.67)	ILCT/MLCT/LLCT
	S4	376.50	3.2931	0.1130	HOMO-1→LUMO+1 (0.50)	LLCT/MLCT
4	S2	380.41	3.2592	0.0789	HOMO→LUMO+1 (0.64)	MLCT/LLCT/LC
	S4	3.5157	352.66	0.2922	HOMO-1→LUMO (0.60)	MLCT/LLCT
5	S1	408.67	3.0339	0.3898	HOMO→LUMO (0.67)	ILCT/MLCT
	S2	399.93	3.1002	0.0785	HOMO-1→LUMO (0.67)	LLCT/MLCT

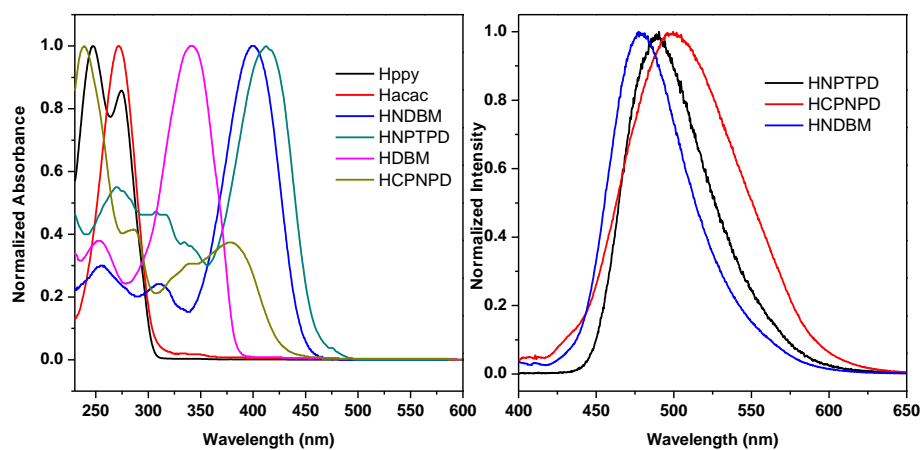


Fig. S1 Absorption (left) and emission (right) spectra of β -diketonate ligands at room temperature in CH_2Cl_2 solution.

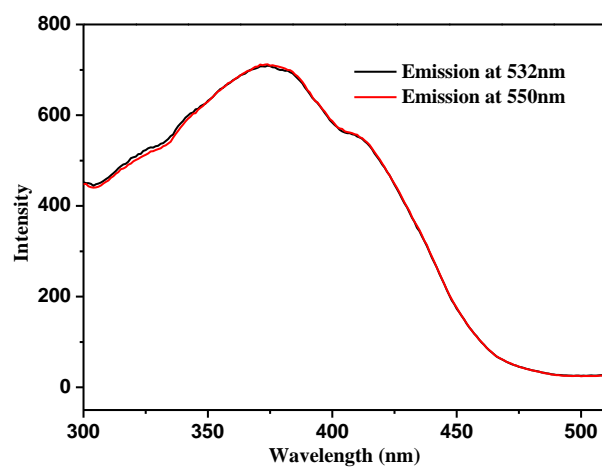


Fig. S2 Excitation spectra of [Pt(ppy)(CPNPD)] at 532 and 550 nm.

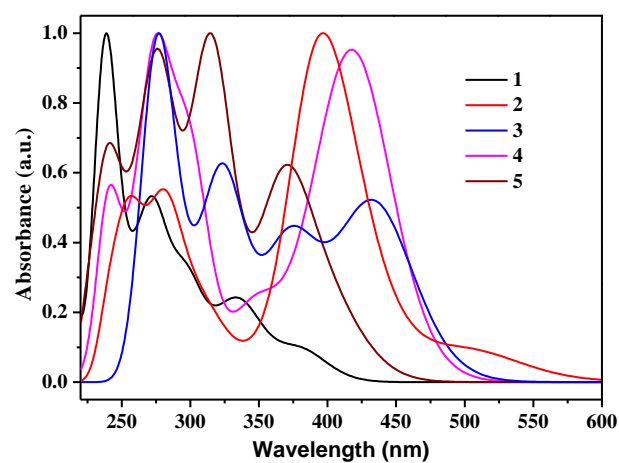


Fig. S3 Calculated absorption spectra of 1-5 at room temperature in CH_2Cl_2 solution.

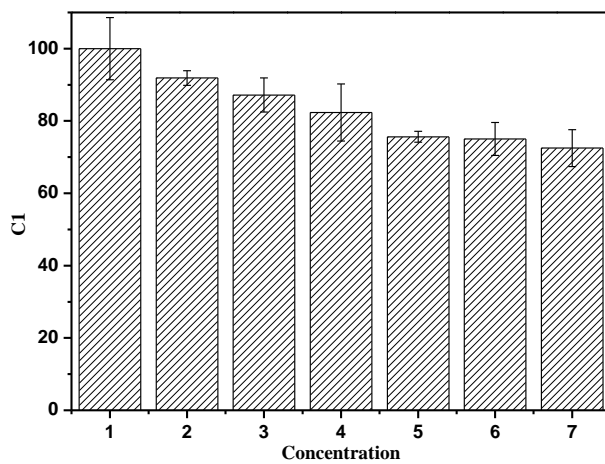


Fig. S4 Viability of KB cells with **1** (from left to right: 0, 3, 6.25, 12.5, 25, 50, 100 μ M).

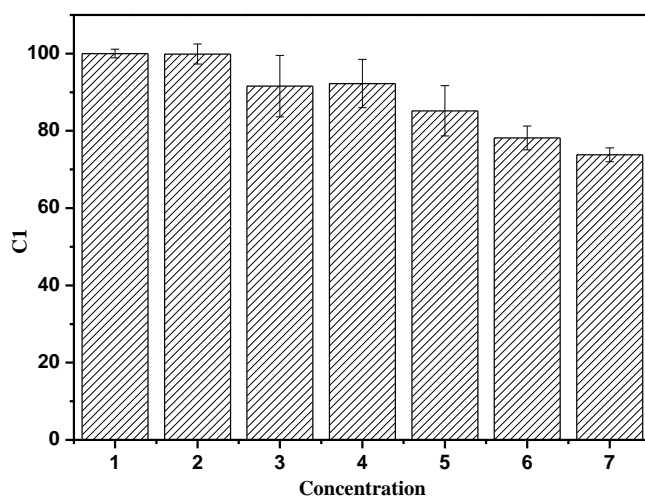


Fig. S5 Viability of KB cells with **2** (from left to right: 0, 3, 6.25, 12.5, 25, 50, 100 μ M).

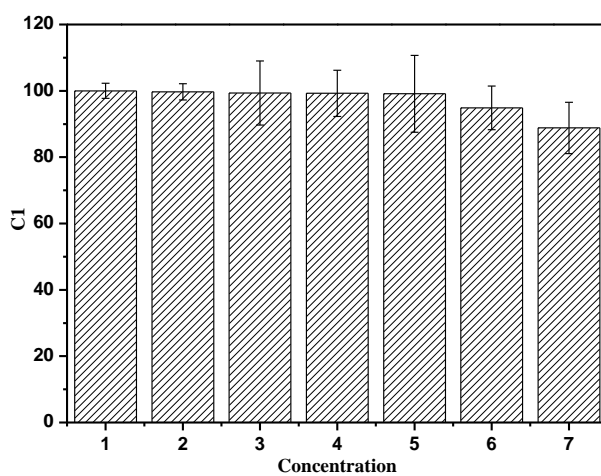


Fig. S6 Viability of KB cells with **3** (from left to right: 0, 3, 6.25, 12.5, 25, 50, 100 μ M).

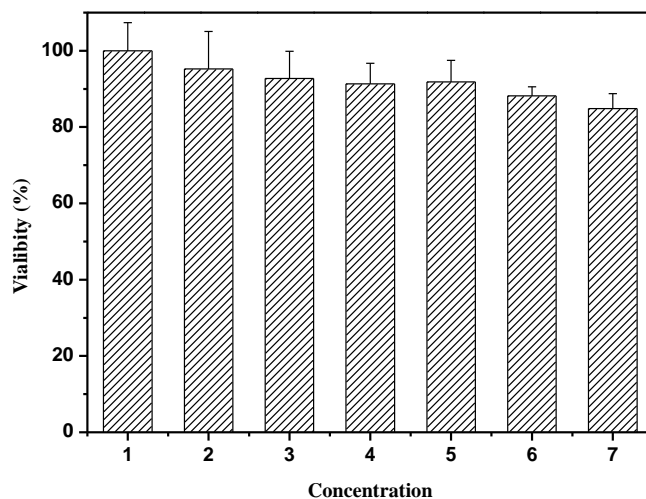


Fig. S7 Viability of KB cells with **4** at 37 °C for 24 h (from left to right: 0, 3, 6.25, 12.5, 25, 50, 100 μ M).

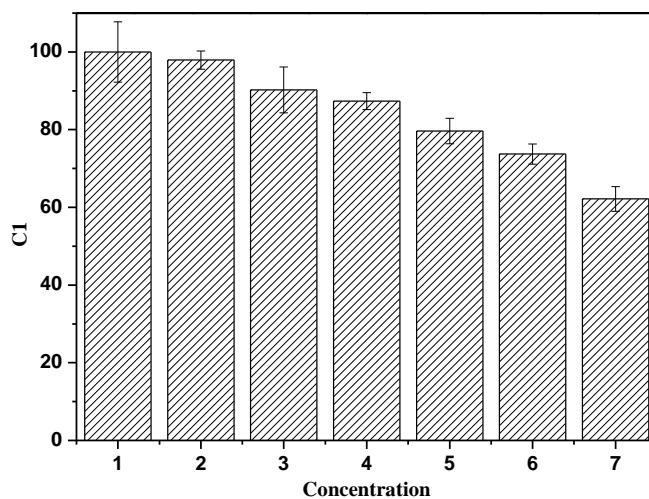


Fig. S8 Viability of KB cells with **5** (from left to right: 0, 3, 6.25, 12.5, 25, 50, 100 μ M).