

Supporting Information

Photophysical and DFT studies on cycloplatinated complexes: modification in luminescence properties by expanding of π -conjugated system

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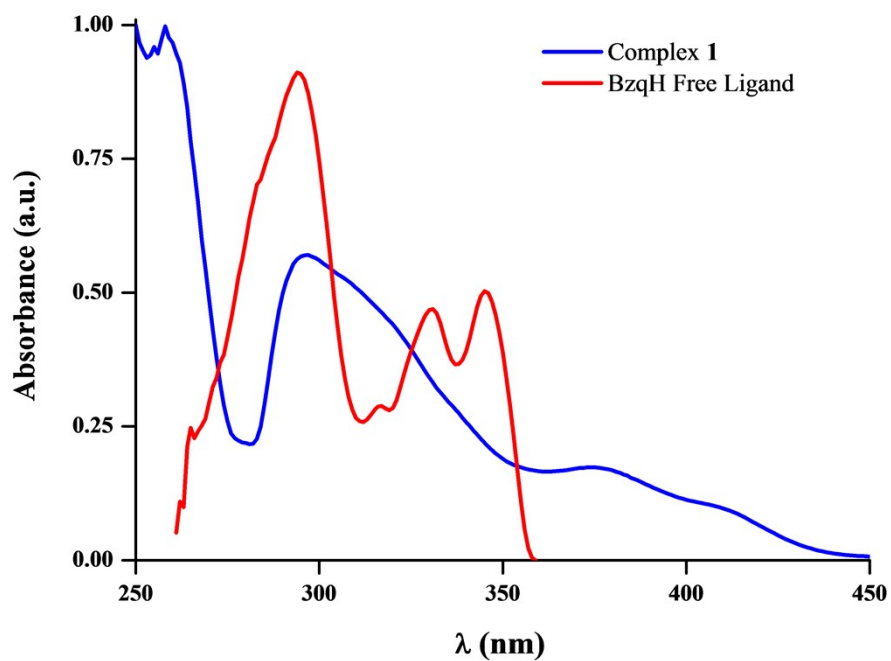


Figure S1. Normalized UV-vis spectra of the complex **1** and free bzqH compound in CH₂Cl₂.

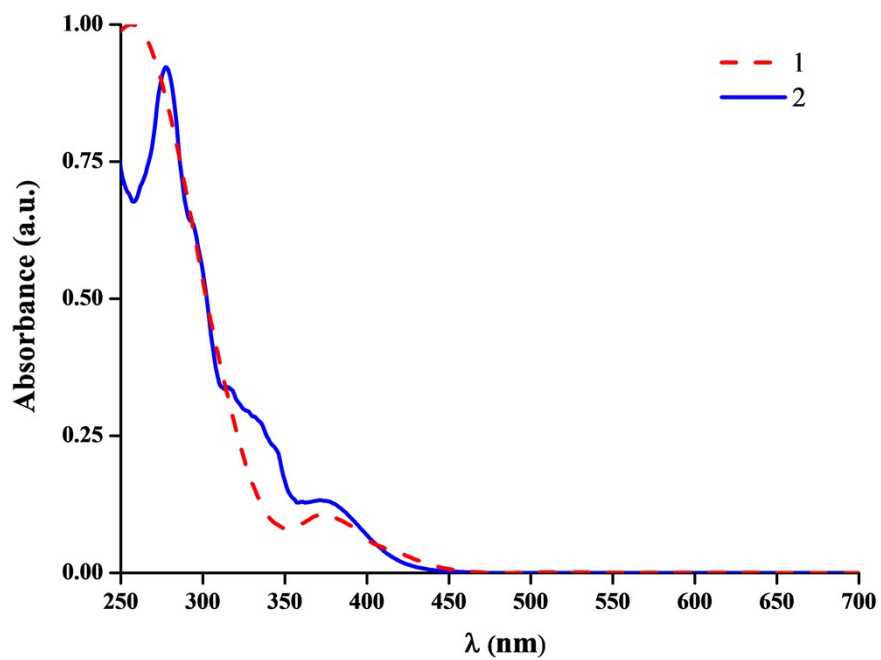


Figure S2. Normalized UV-vis spectra of the complexes **1** and **2** in 2-MeTHF ($5 \times 10^{-5} \text{ M}$)

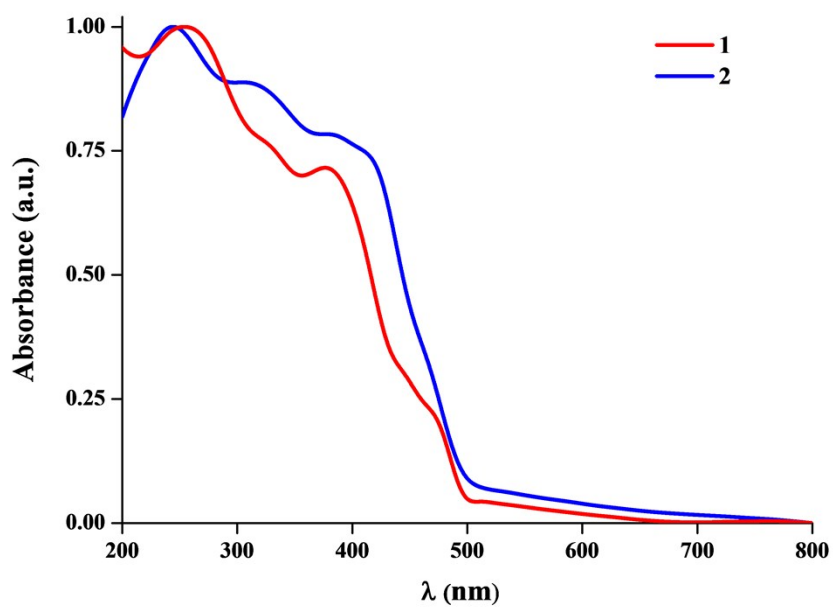


Figure S3. Normalized diffuse reflectance UV-vis spectra of the complexes **1** and **2** in solid state.

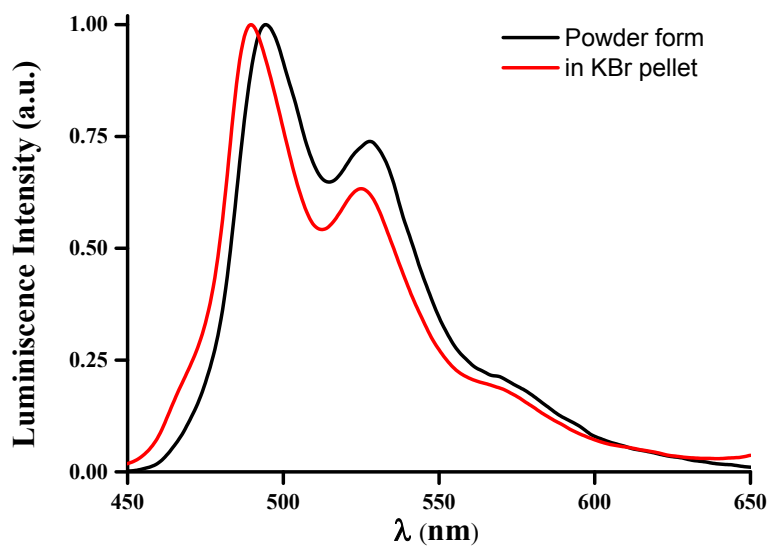


Figure S4. Normalized emission spectra of the complex **1** in solid state at different form.

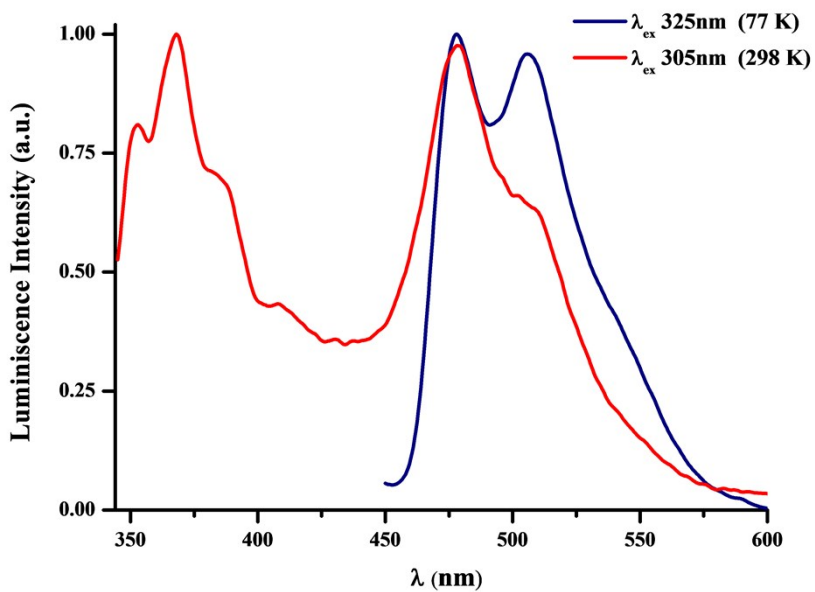


Figure S5. Normalized emission spectra of the complex **1** in CH_2Cl_2 solution (5×10^{-5} M) at 298 and 77 K.

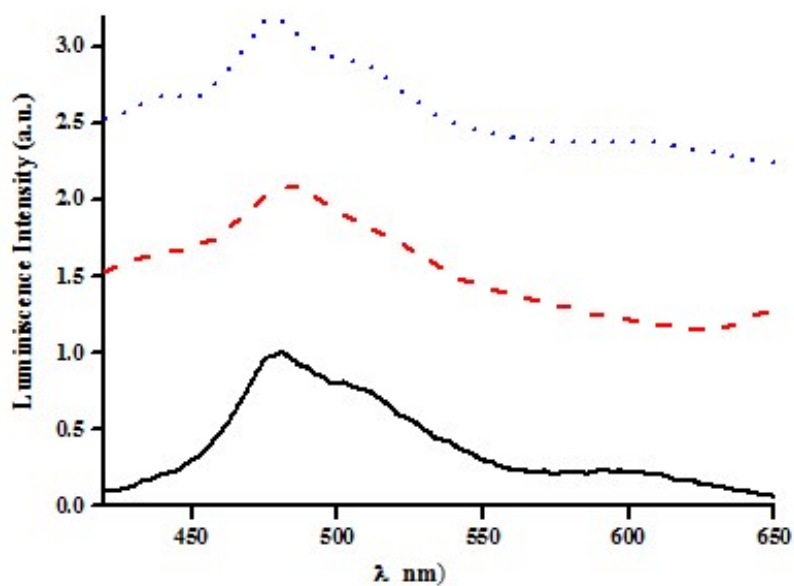


Figure S6. Normalized emission spectra of complex **1** in CH_2Cl_2 at 298 K at several concentrations (10^{-3}M , solid line; 10^{-4}M , dashed line and $5 \times 10^{-5}\text{M}$, dotted line).

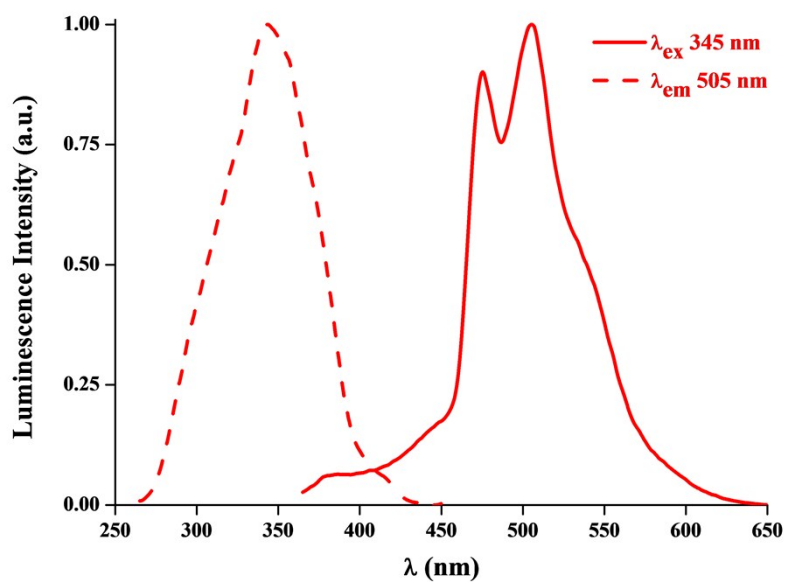


Figure S7. Normalized excitation (dotted lines) and emission spectra (solid lines) of the complex **2** in CH_2Cl_2 solution (10^{-3}M) at 298 K.

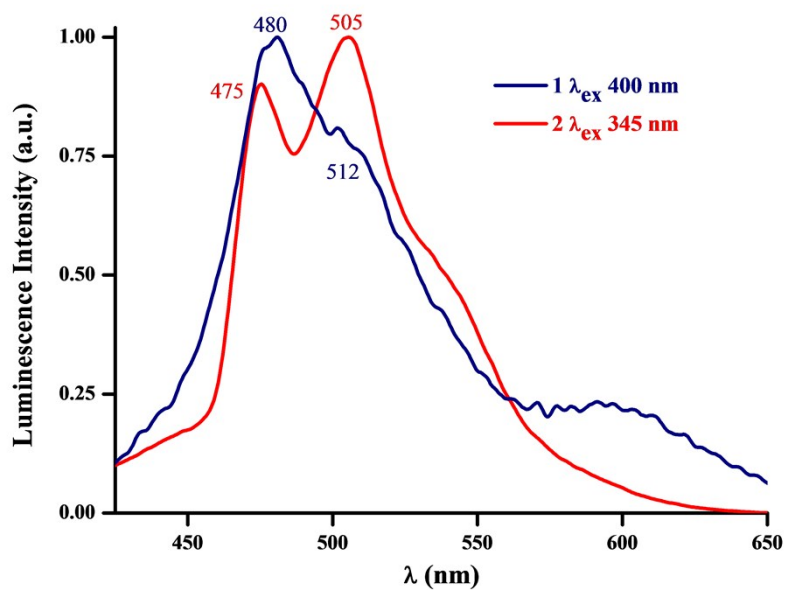


Figure S8. Normalized emission spectra of the complexes **1** and **2** in CH_2Cl_2 solution (10^{-3} M) at 298 K.

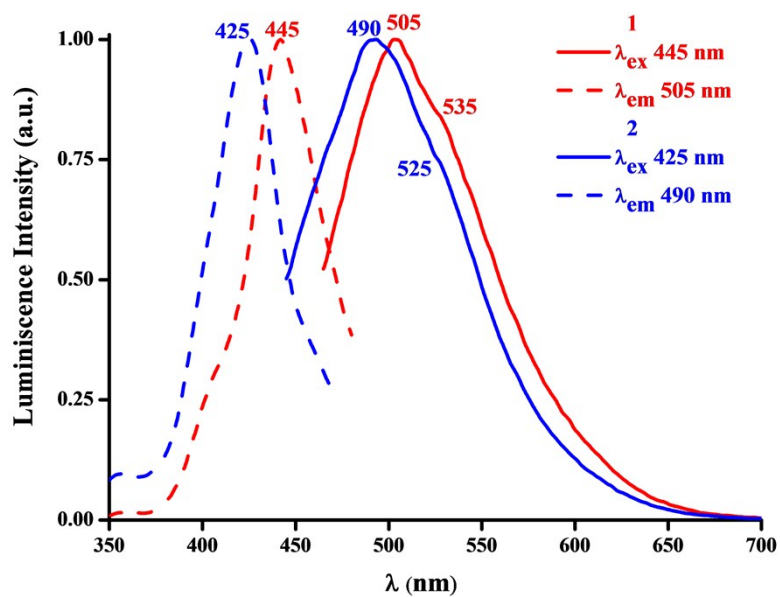


Figure S9. Normalized excitation spectra (dotted lines) and emission spectra (solid lines) of the complexes **1** and **2** in 2-MeTHF solution (5×10^{-5} M) at 298 K.

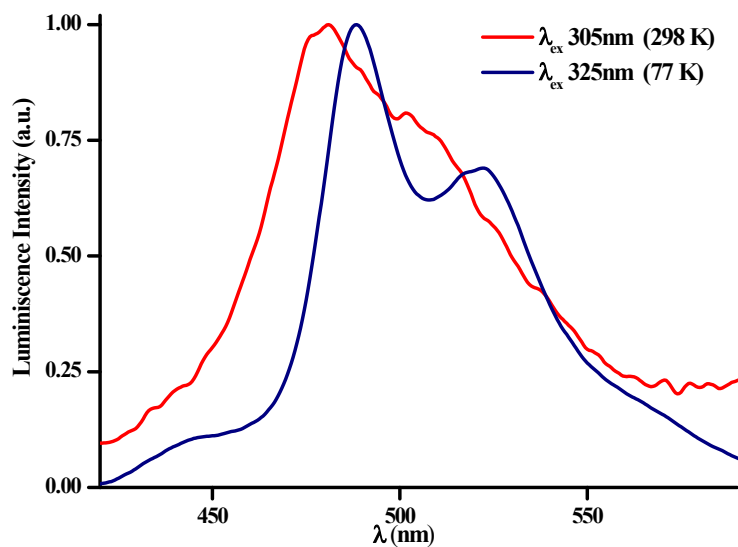


Figure S10. Normalized emission spectra of the complex **1** in CH₂Cl₂ solution (10⁻³ M) at 298 and 77 K.

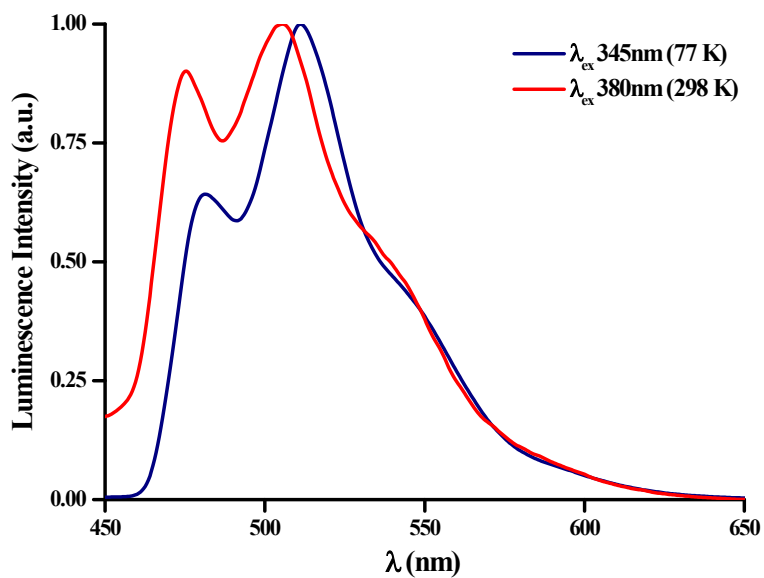


Figure S11. Normalized emission spectra of the complex **2** in CH₂Cl₂ solution (10⁻³ M) at 298 and 77 K.

Table S1. Composition (%) of frontier MOs in the ground state (S_0) for the complex **1**, [Pt(p -MeC₆H₄)(bzq)(SMe₂)], in gas phase

MO orbitals	Pt	SMe ₂	bzq	p -MeC ₆ H ₄
L + 5	19	17	23	42
L + 4	1	4	7	88
L + 3	13	58	22	7
L + 2	5	12	76	6
L + 1	2	8	88	2
LUMO	2	1	95	2
HOMO	27	3	5	65
H - 1	31	3	65	2
H - 2	80	1	10	9
H - 3	54	0	34	12
H - 4	15	1	2	81
H - 5	38	0	57	5
H - 6	45	2	52	1

Table S2. Composition (%) of frontier MOs in ground state (S_0) for complex **2**, [Pt(p -MeC₆H₄)(ppy)(SMe₂)], in gas phase.

MO orbitals	Pt	SMe ₂	ppy	p -MeC ₆ H ₄
L + 6	29	17	31	23
L + 5	11	41	40	8
L + 4	18	19	17	46
L + 3	3	5	7	85
L + 2	12	52	27	9
L + 1	1	2	97	0
LUMO	6	2	89	3
HOMO	27	3	5	65
H - 1	42	3	54	1
H - 2	81	1	9	9
H - 3	52	0	35	12
H - 4	16	1	2	80
H - 5	38	0	56	6