

Electronic Supporting Information for:

Excited State Processes of Dinuclear Pt(II) Complexes Bridged by 8-hydroxyquinoline

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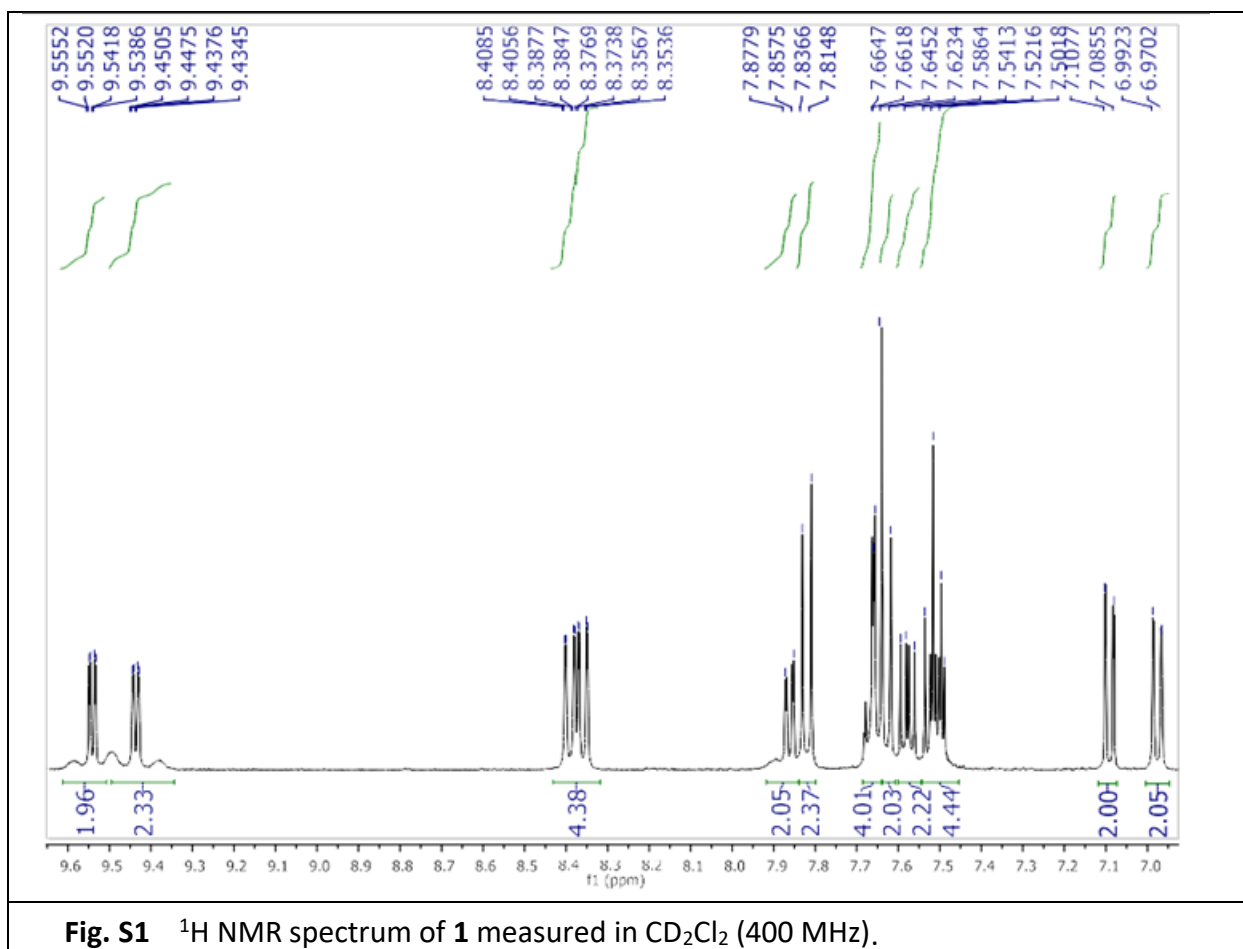


Fig. S1 ¹H NMR spectrum of **1** measured in CD₂Cl₂ (400 MHz).

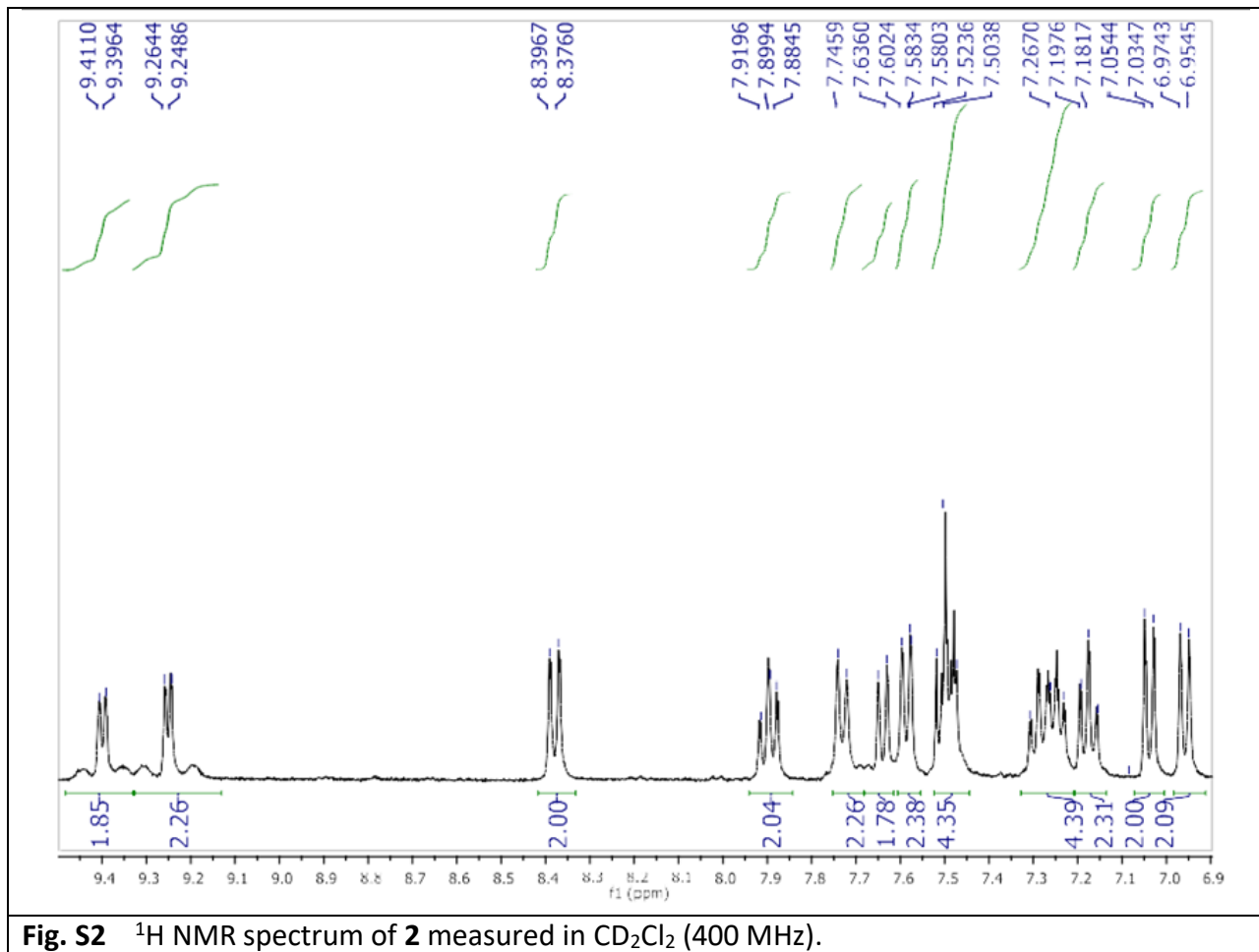


Fig. S2 ¹H NMR spectrum of **2** measured in CD₂Cl₂ (400 MHz).

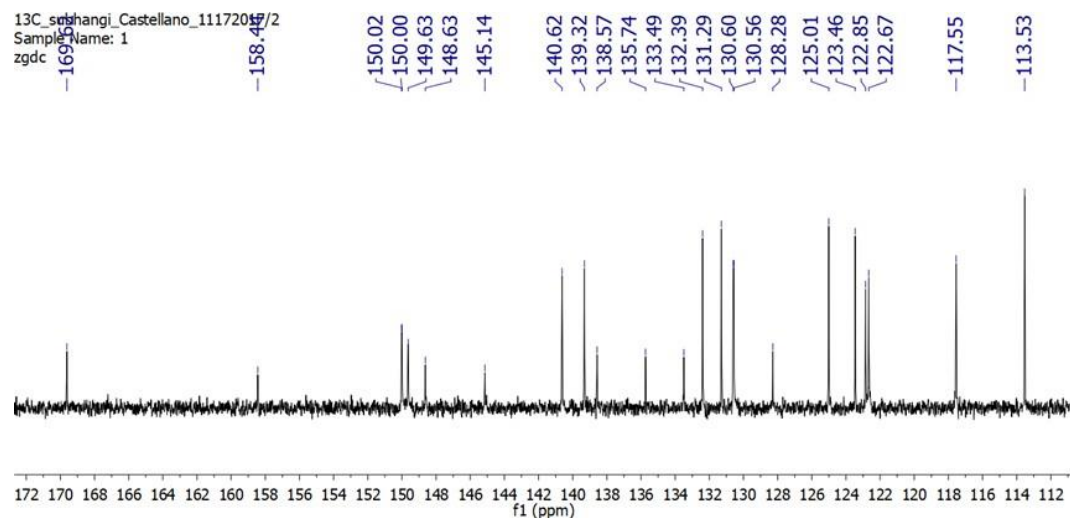


Fig. S3 ^{13}C NMR spectrum of **1** measured in CD_2Cl_2 (100 MHz).

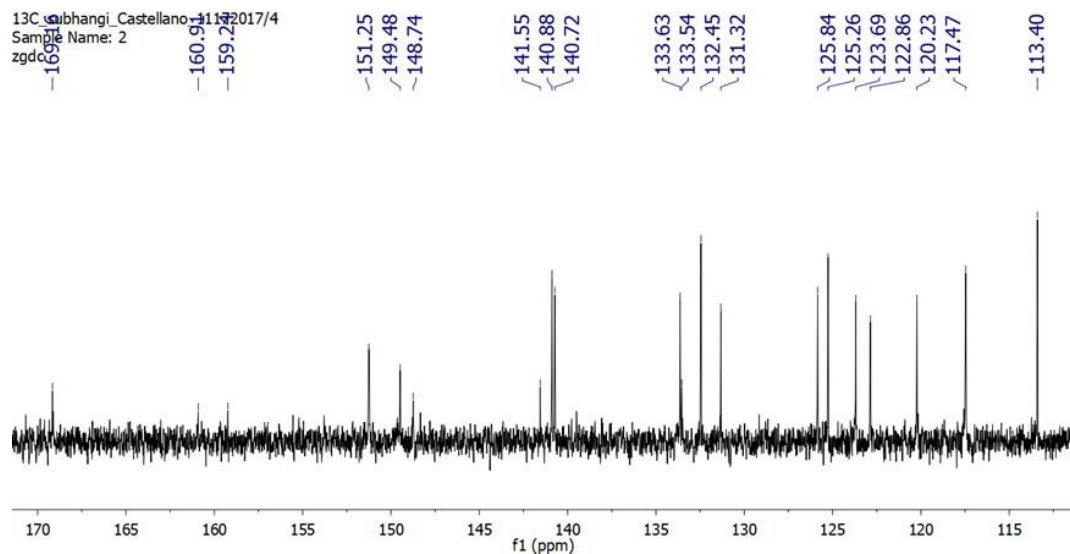


Fig. S4 ^{13}C NMR spectrum of **2** measured in CD_2Cl_2 (100 MHz).

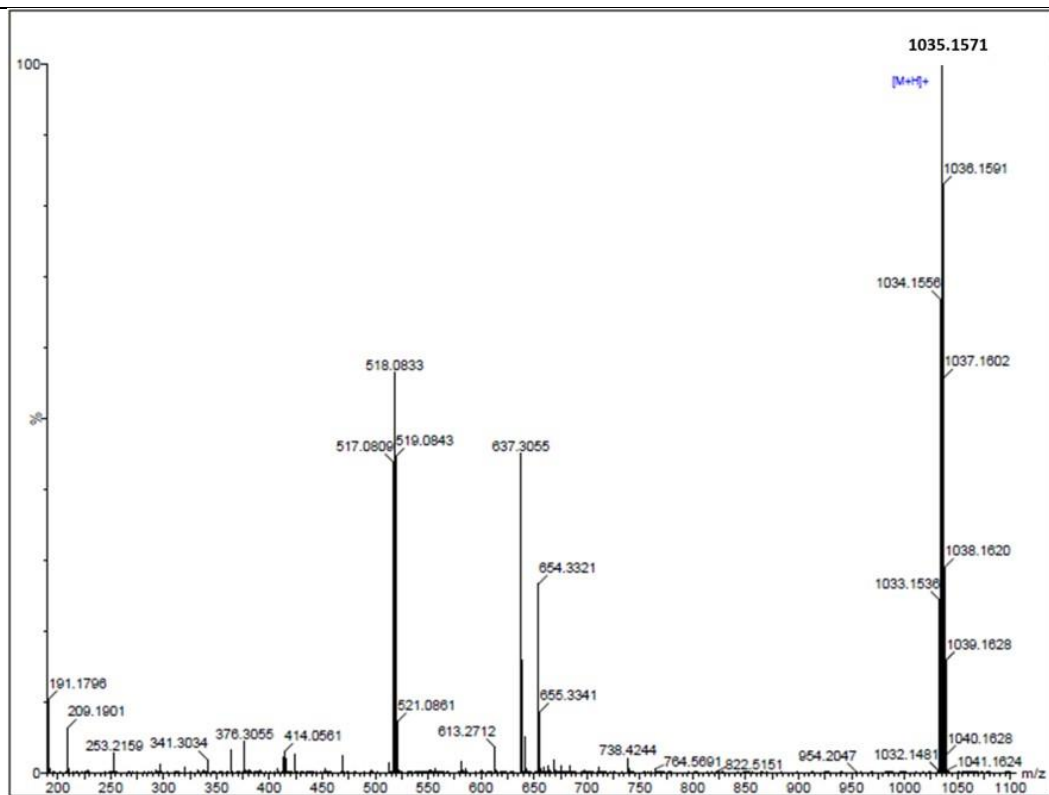


Fig. S5 High resolution mass spectrum of **1**. The calculated mass for [M+H]⁺ is 1035.1586.

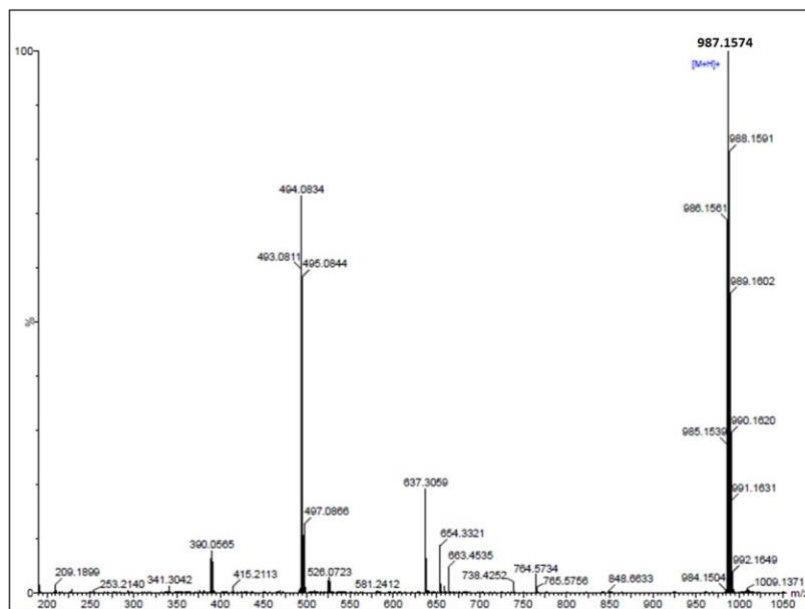


Fig. S6 High resolution mass spectrum of **2**. The calculated mass for $[M+H]^+$ is 987.1586.

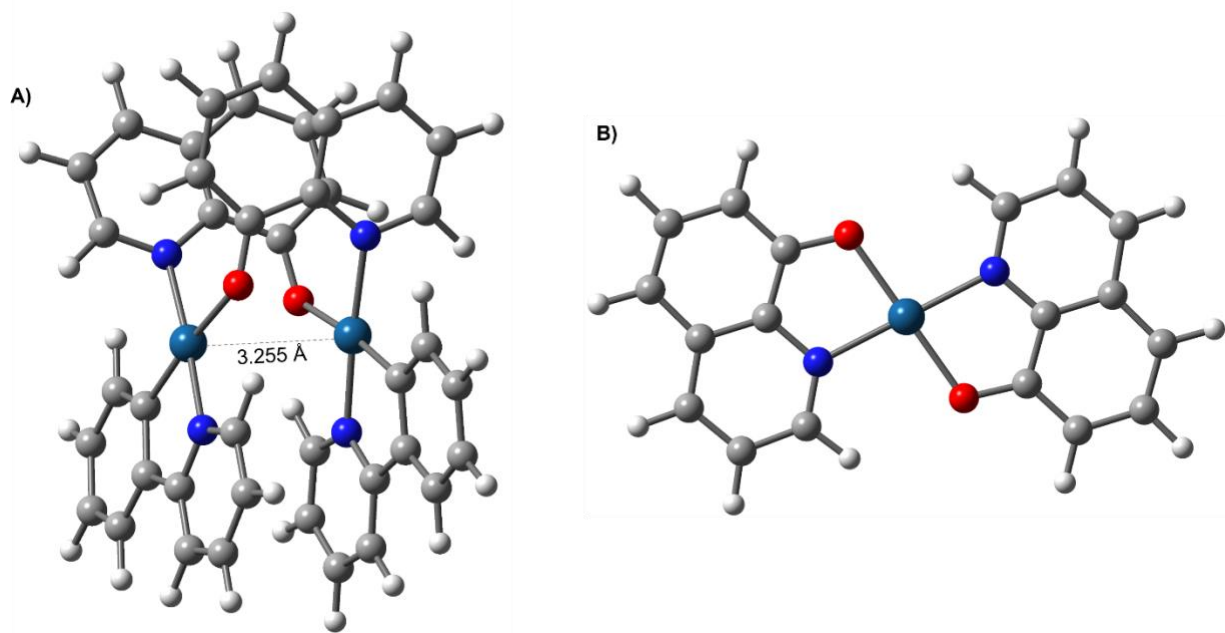


Fig. S7 DFT optimized structures of **2** (a) and **3** (b), calculated at the PCM-PBE0-D3/Def2-SVP/SDD level of theory

Table S1 Selected bond distances in Ångstroms as well as bond and dihedral angles in Degrees from DFT optimized structures of **1** and **2**, where bridging nitrogens denoted (B) and cyclometalating (C). Calculated at the PCM-PBE0-D3/Def2-SVP/SDD level of theory.

	1	2
Pt-Pt	3.243	3.255
Pt-N (B)	2.061	2.066
Pt-N (C)	2.023	2.012
Pt-O	2.142	2.151
N(B)-Pt-N(C)	176.9	176.2
N-Pt-Pt-N	50.312	48.345

Table S2 Selected bond distances in Ångstroms and bond angles in degrees from the DFT optimized structure of **3** in comparison with values from the reported crystal structure.¹

	3	Crystal Structure
Pt-N	2.01	1.993
Pt-O	2.018	2.014
N-Pt-N	180	180
O-Pt-O	180	180

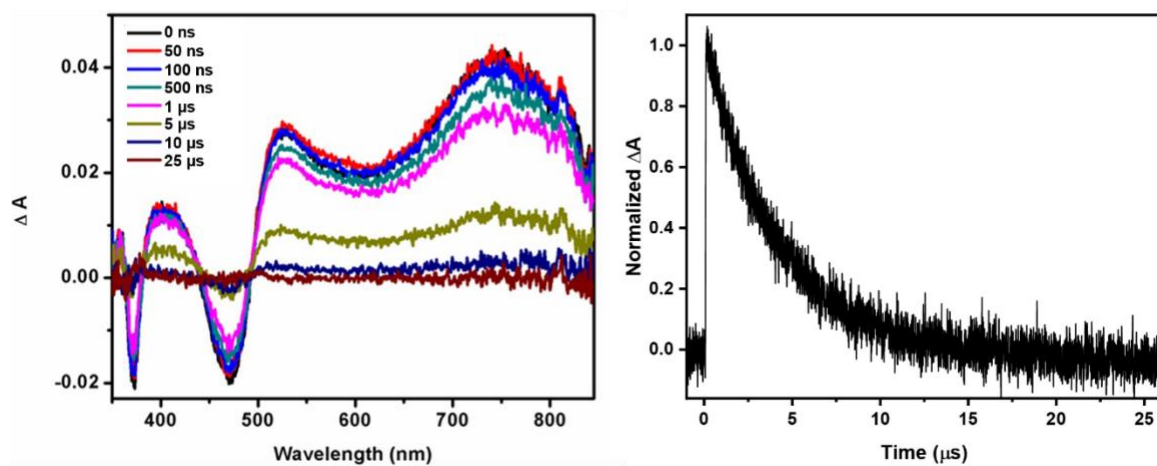


Fig. S8 Excited state absorption difference spectra of [Pt(ppy)(μ -8HQ)]₂ (**2**) in THF with 490 nm pulsed excitation (2 mJ/pulse, 7 nm fwhm). The sample was deaerated for 30 minutes with bubble-degassing. (B) Single exponential kinetic fit for the decay profile at 530 nm.

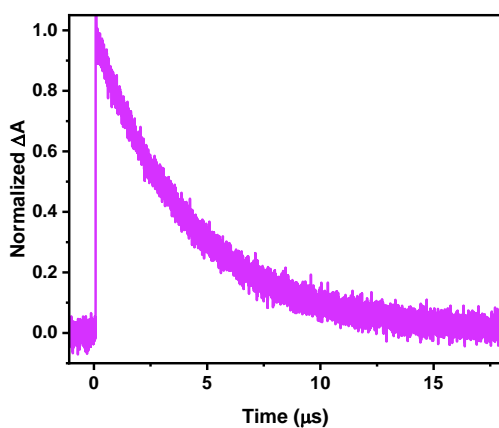


Fig. S9 Single exponential emission decay of [Pt(ppy)(μ -8HQ)]₂ (**2**) in THF with 500 nm pulsed excitation (2 mJ/pulse, 7 nm fwhm). The sample was prepared in an air-free glove box under N₂.

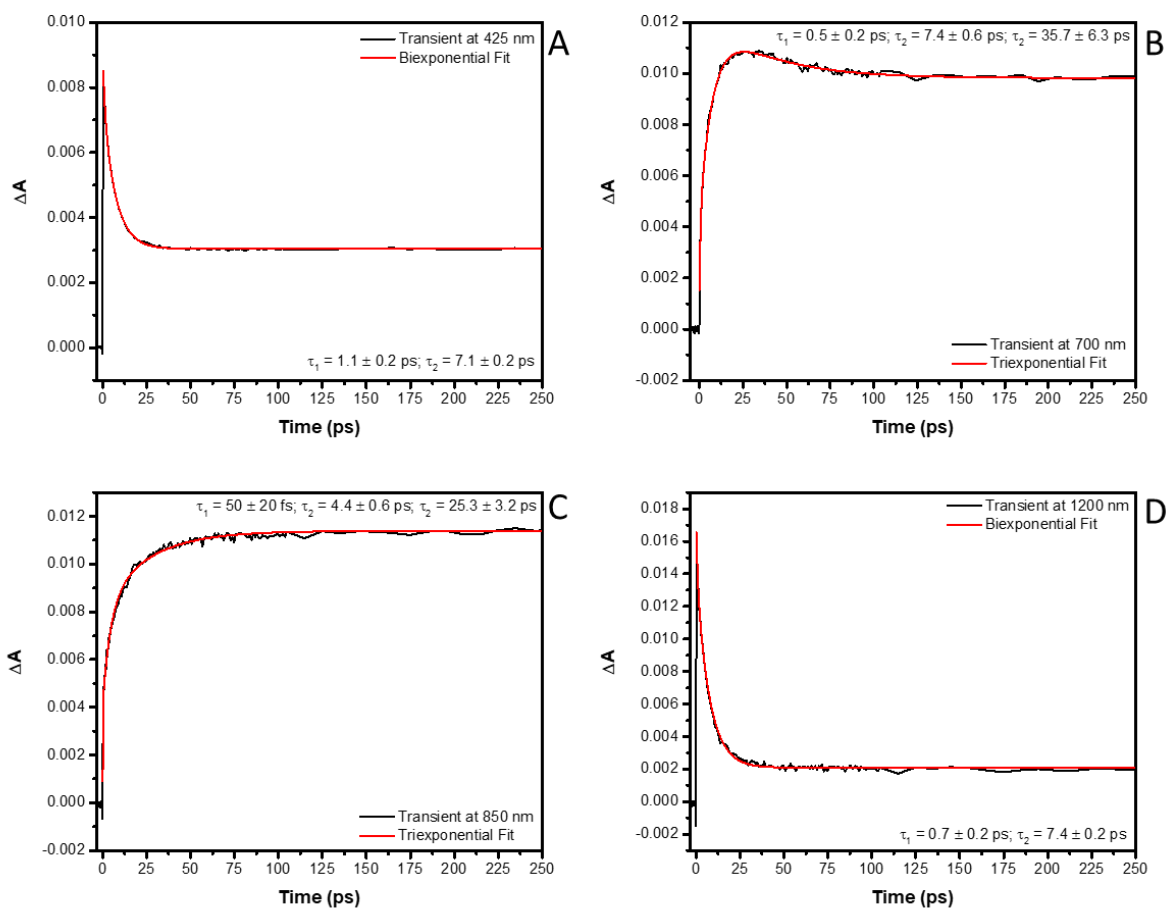


Fig. S10 Ultrafast kinetic analysis of $[\text{Pt}(\text{bzq})(\mu\text{-8HQ})]_2$ (**1**) at 425 nm (A), 700 nm (B), 850 nm (C), and 1200 nm (D) in THF with 500 nm pulsed laser excitation (100 fs fwhm).

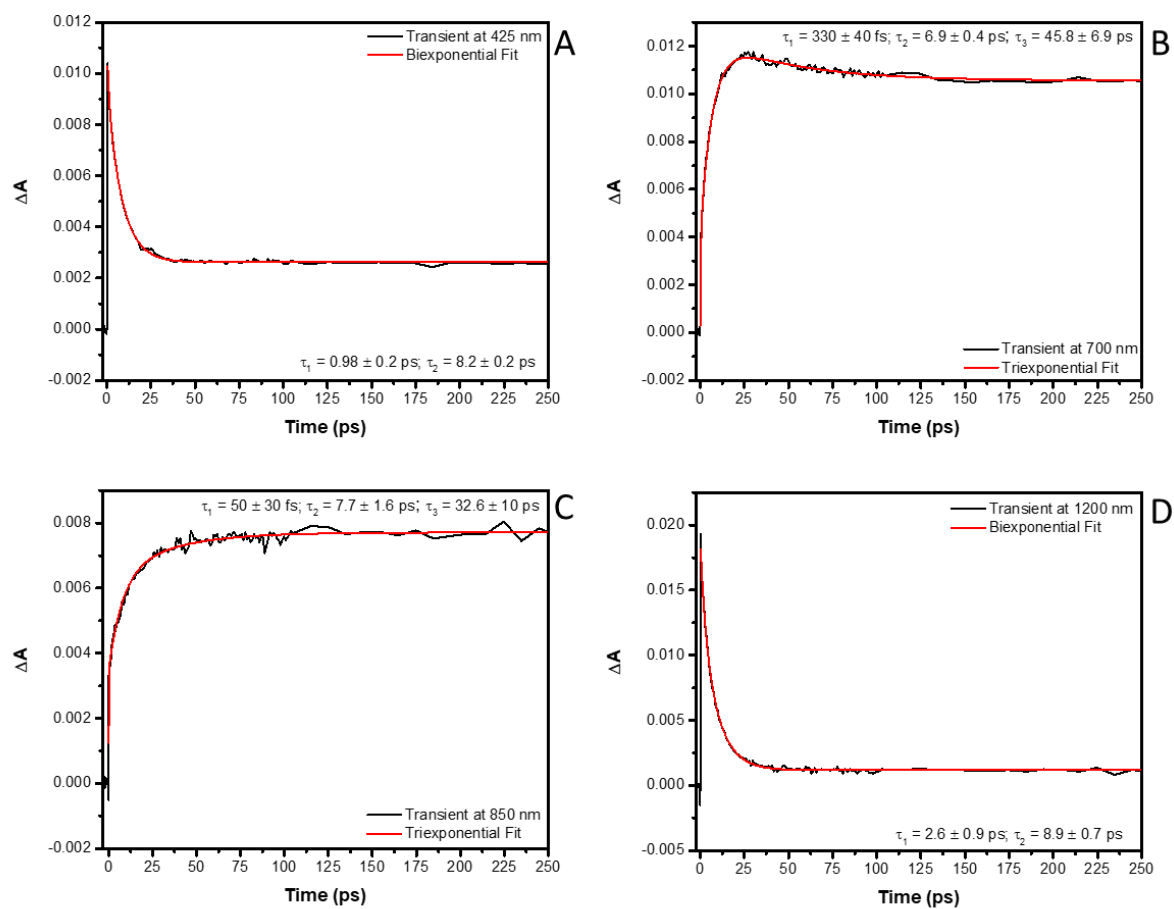


Fig. S11 Ultrafast kinetic analysis of $[Pt(ppy)(\mu-8HQ)]_2$ (**2**) at 425 nm (A), 700 nm (B), 850 nm (C), and 1200 nm (D) in THF with 500 nm pulsed excitation (100 fs fwhm).

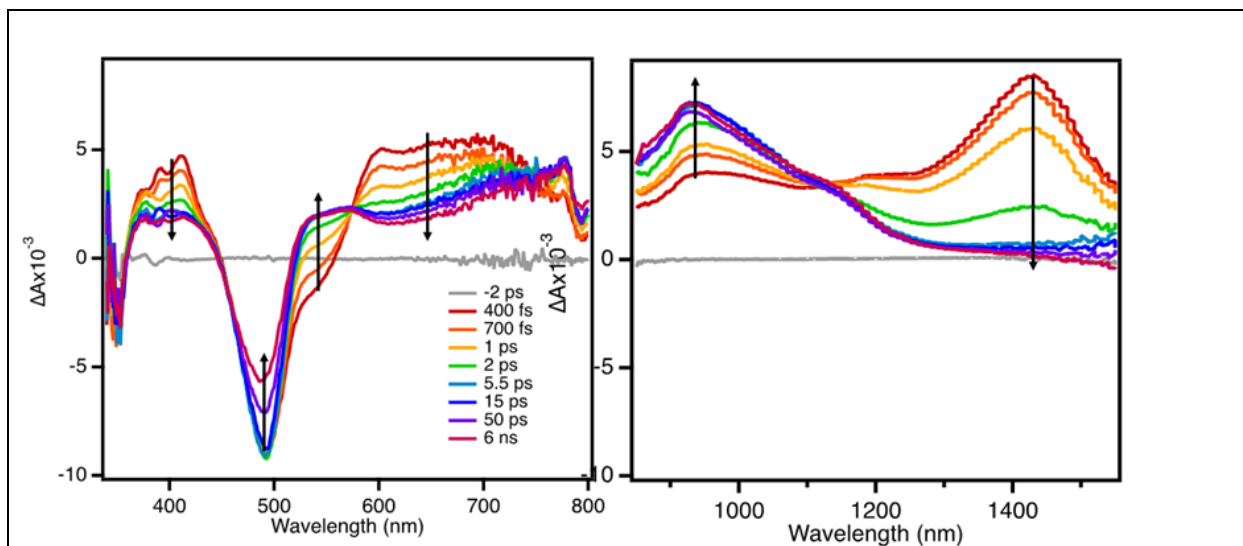


Fig. S12 Ultrafast difference spectra of Pt(8-HQ)₂ after photoexcitation at 500 nm in THF (100 fs fwhm).

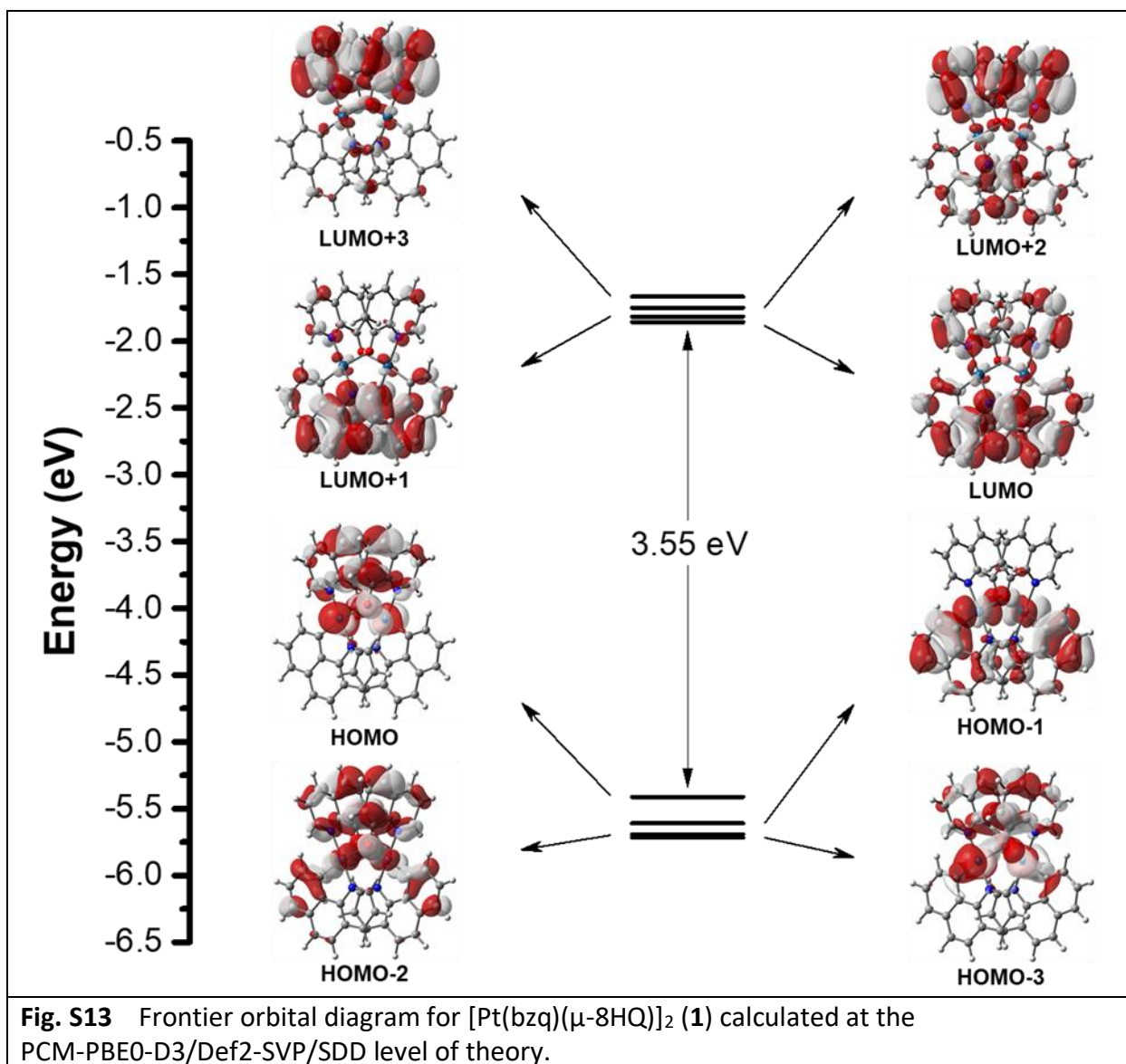


Fig. S13 Frontier orbital diagram for $[\text{Pt}(\text{bzq})(\mu\text{-8HQ})]_2$ (**1**) calculated at the PCM-PBE0-D3/Def2-SVP/SDD level of theory.

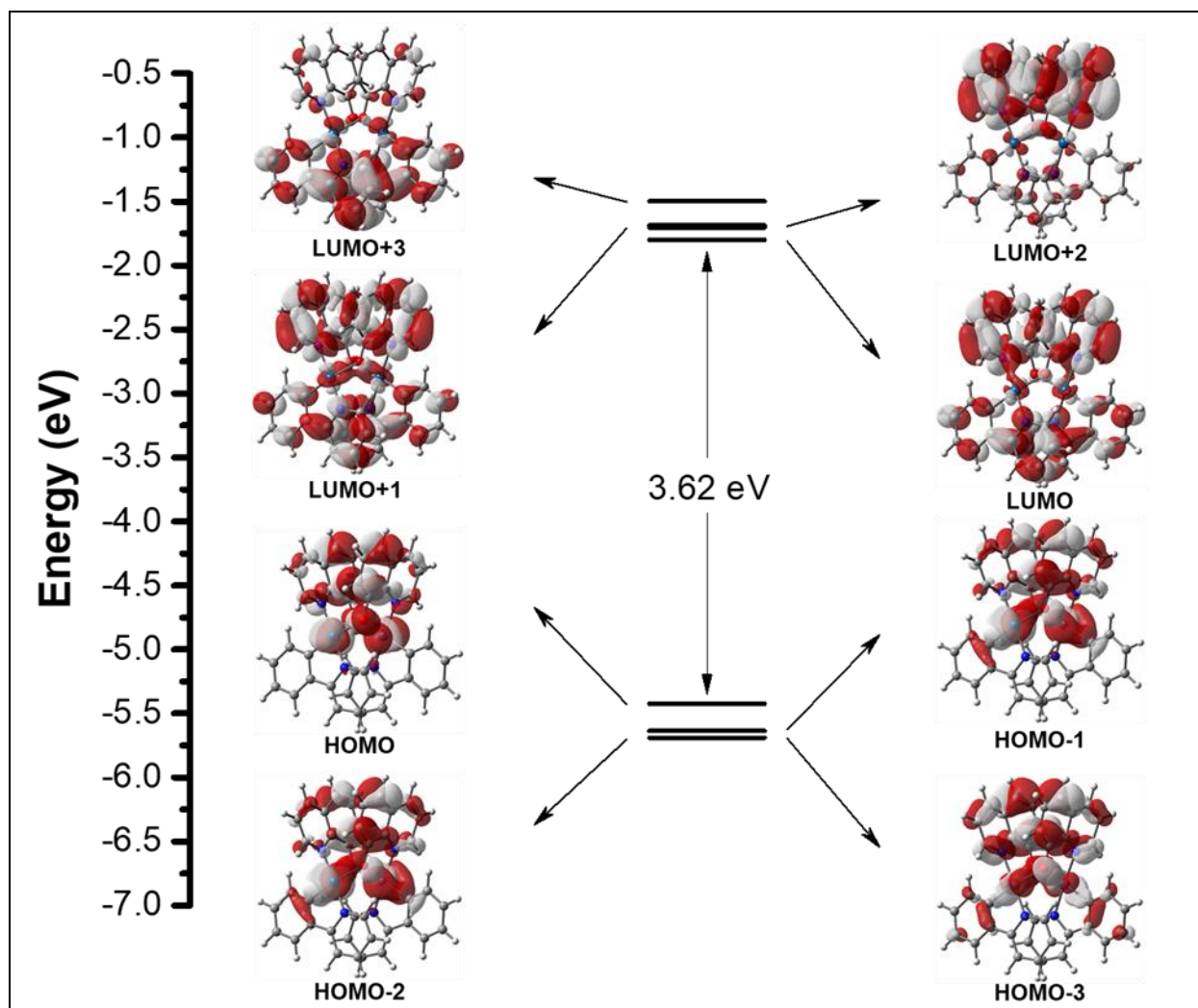


Fig. S14 Frontier orbital diagram for $[\text{Pt}(\text{ppy})(\mu\text{-8HQ})]_2$ (**2**) calculated at the PCM-PBE0-D3/Def2-SVP/SDD level of theory.

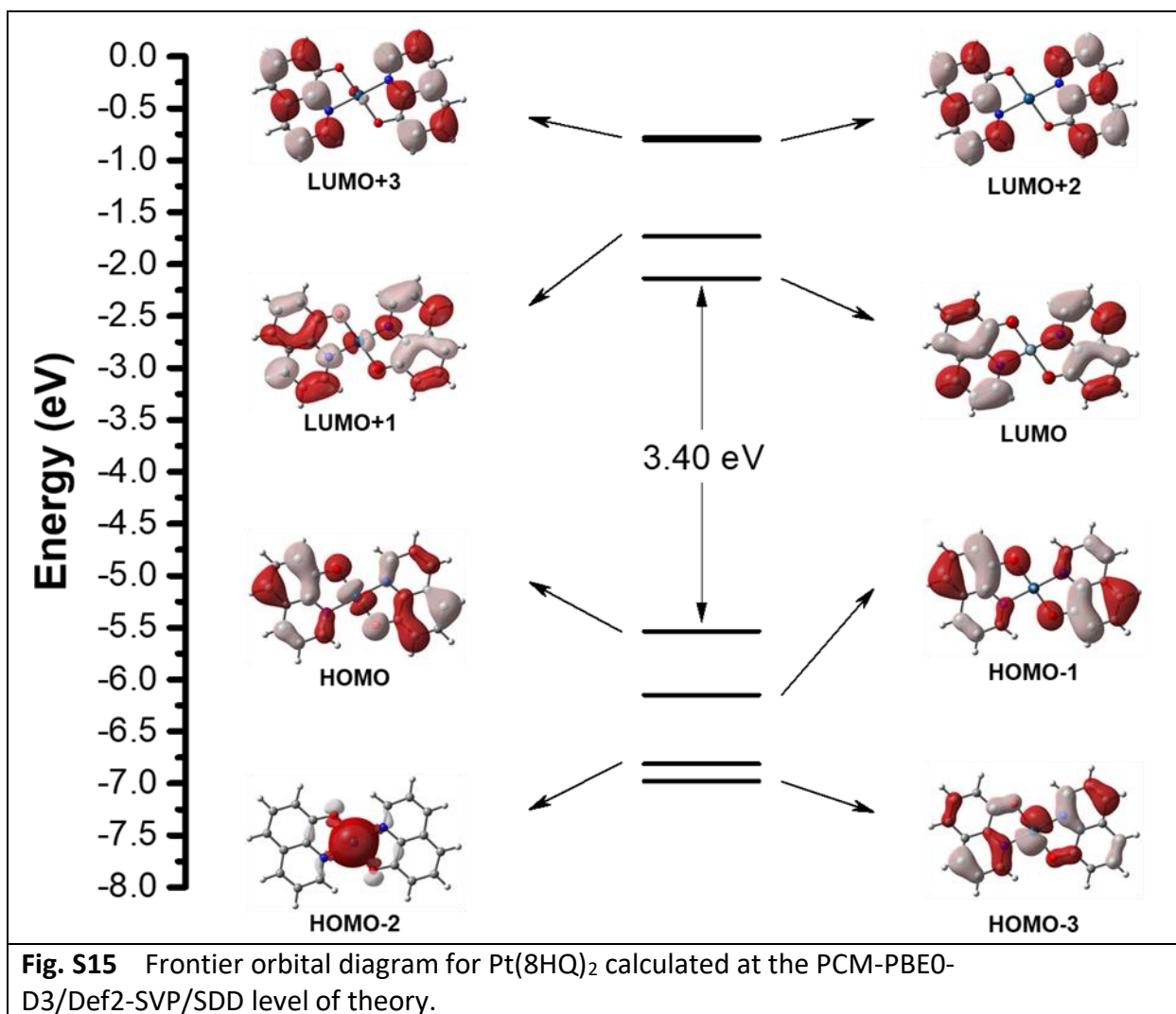


Fig. S15 Frontier orbital diagram for Pt(8HQ)₂ calculated at the PCM-PBE0-D3/Def2-SVP/SDD level of theory.

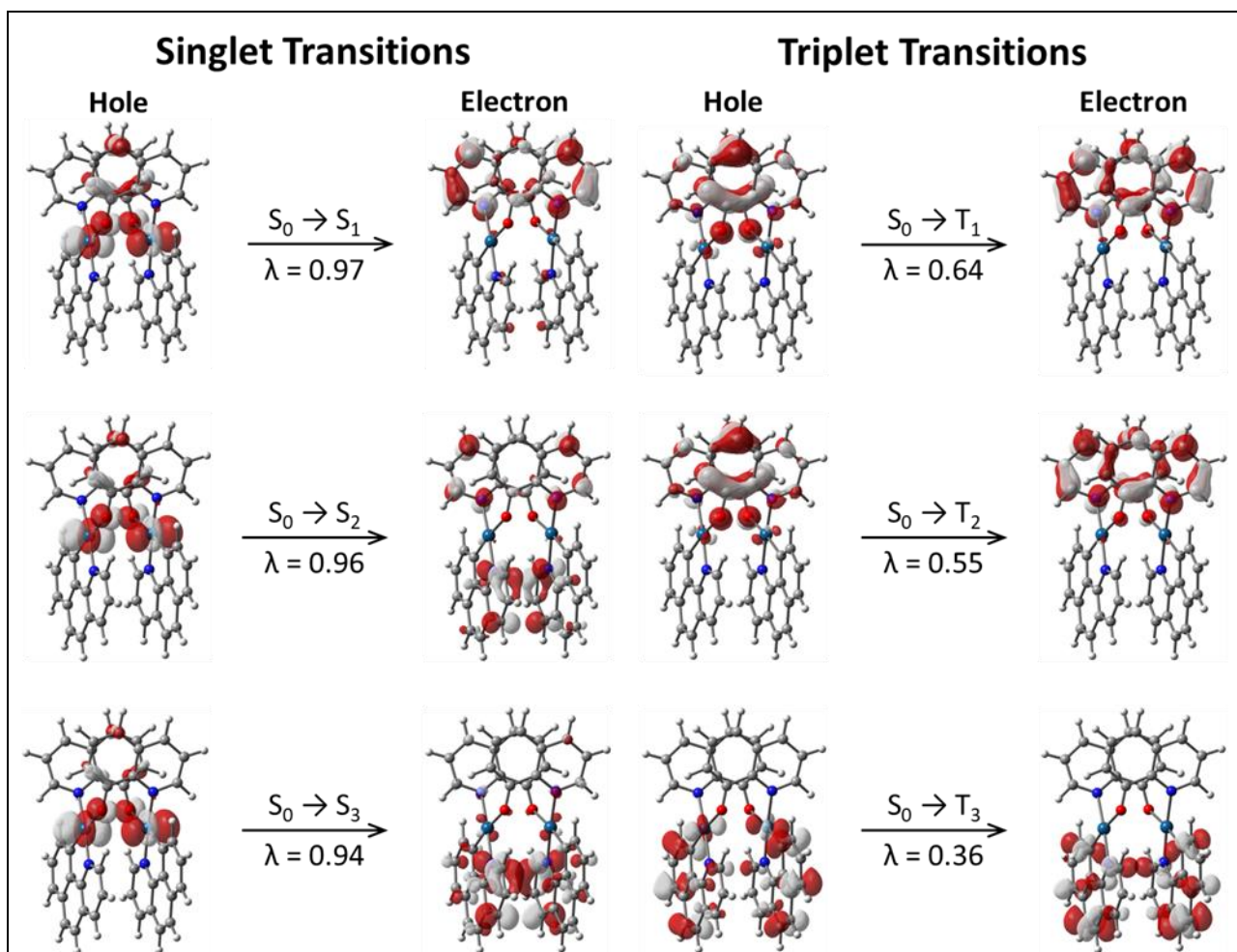
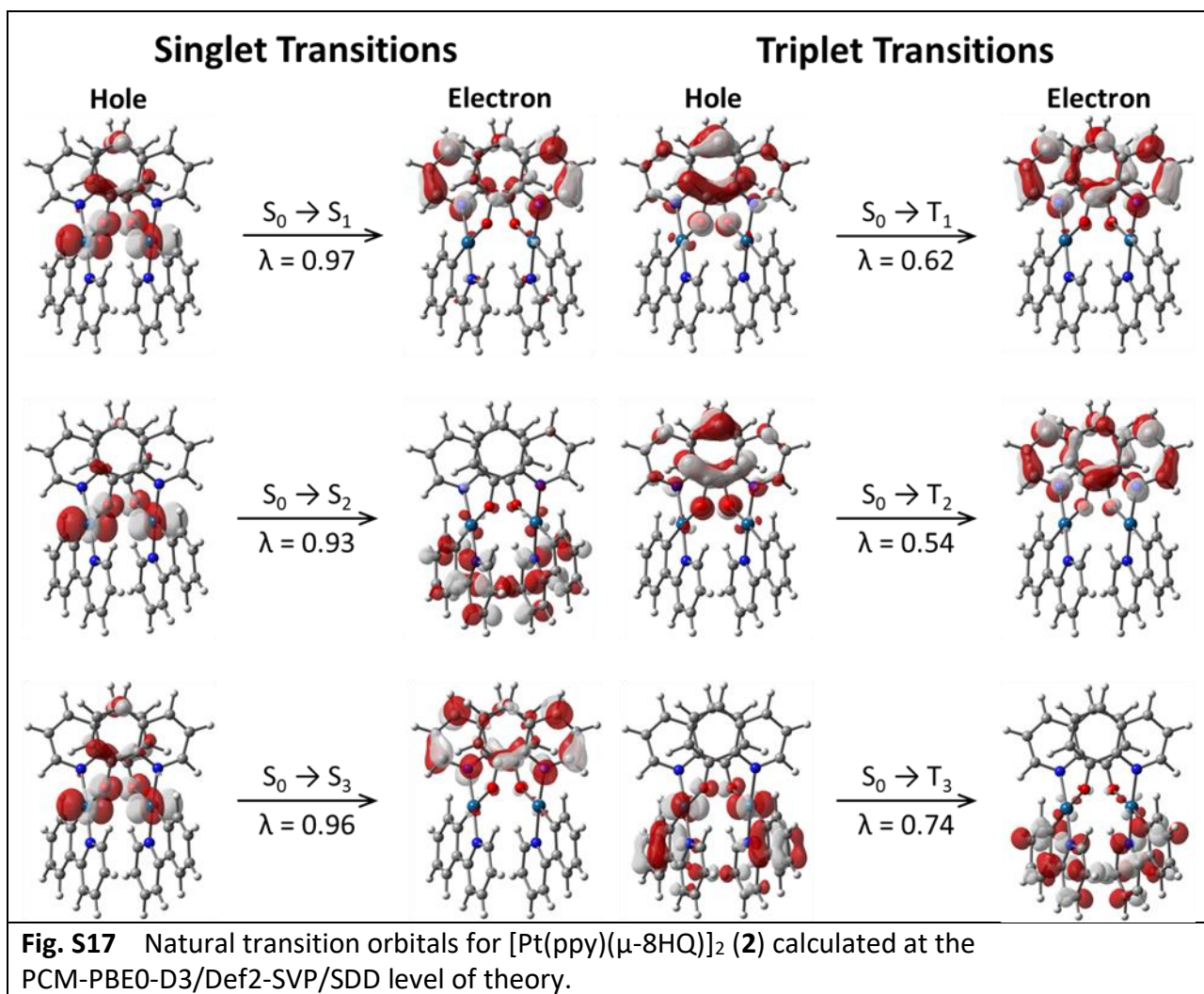
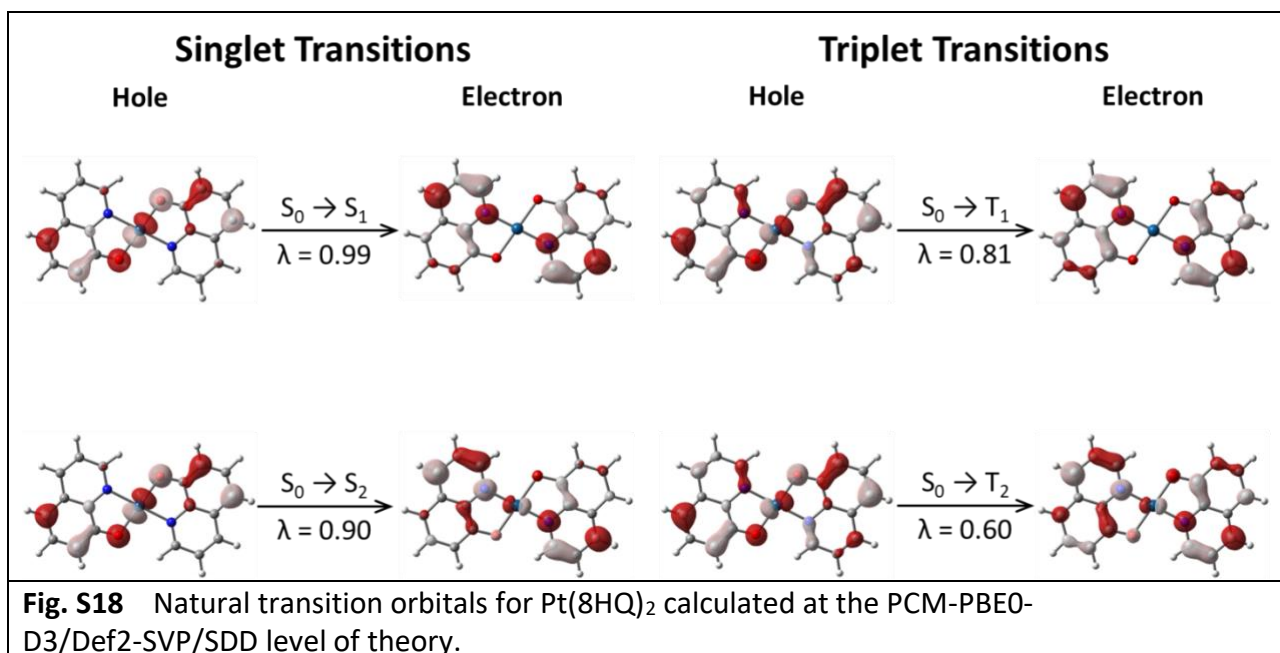


Fig. S16 Natural transition orbitals for [Pt(bzq)(μ-8HQ)]₂ (**1**) calculated at the PCM-PBE0-D3/Def2-SVP/SDD level of theory.





References

- (1) M. Kato, Y. Ogawa, M. Kozakai and Y. Sugimoto, *Acta. Cryst.*, 2002, **C58**, m147-m149