DFT studies of dimethylaminophenyl-substituted phthalocyanine and of its silver complexes

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Supplementary information

Figure S1. UV-vis spectra of neutral dmaphPcAg (full line) and dmaphPcH$_2$ (dashed line) in CHCl$_3$.

Figure S2. Time dependence of absorption spectra during photolysis of [dmaphPcAg]^0 under LED@385 nm irradiation.

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Figure S18. TD-DFT calculated electron transitions in ^{1}[dmaphPcH$_2$]^0 in CHCl$_3$.

Figure S19. TD-DFT calculated electron transitions in ^{1}[dmaphPcH]$^-$ in CHCl$_3$.

Figure S20. TD-DFT calculated electron transitions in ^{2}[dmaphPcH]^0 in CHCl$_3$.

Figure S21. TD-DFT calculated electron transitions in ^{1}[dmaphPc]$^{2-}$ in CHCl$_3$.

Figure S22. TD-DFT calculated electron transitions in ^{2}[dmaphPc]$^-$ in CHCl$_3$.
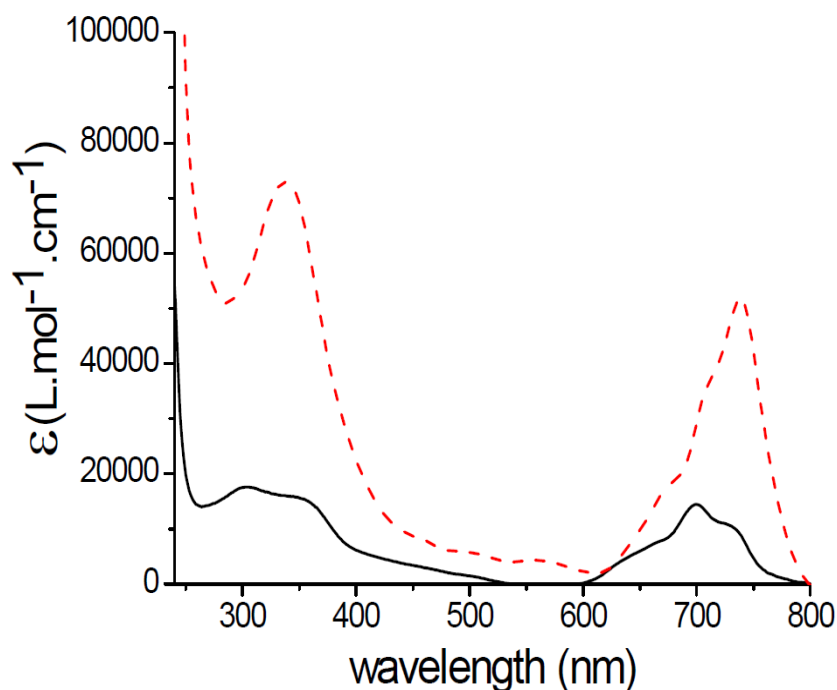
References

Figure S1. UV-vis spectra of neutral dmaphPcAg (full line) and dmaphPcH$_2$ (dashed line) in CHCl$_3$. Reproduced from Ref. [1] with permission from the Royal Society of Chemistry.
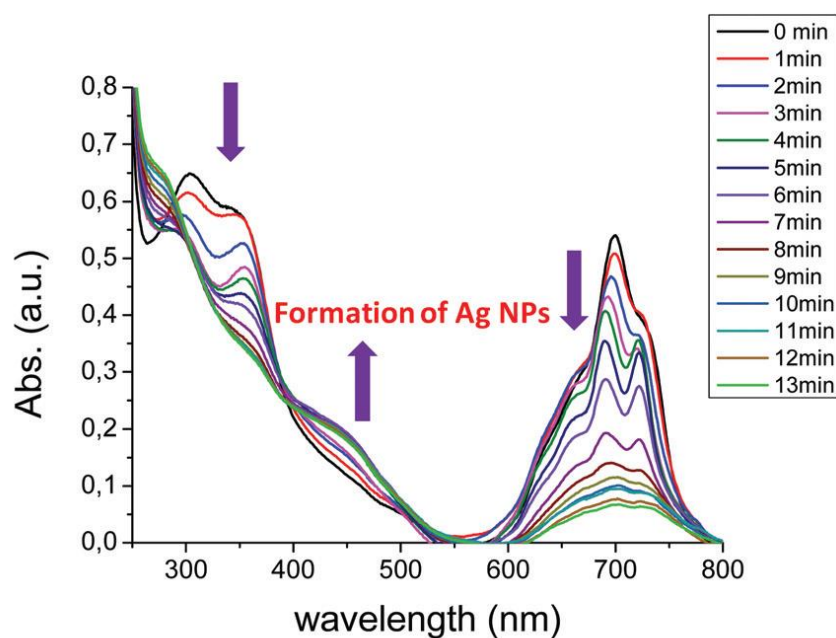

Figure S2. Time dependence of absorption spectra during photolysis of [dmaphPcAg]^0 under LED@385 nm irradiation. LED@385 nm intensity = 470 mW cm^{-2}. Concentration of [dmaphPcAg]^0 = 3.8×10^{-5} M. Solvent = CHCl$_3$. Reproduced from Ref. [1] with permission from the Royal Society of Chemistry.

Figure S3. DFT optimized structure of ^{2}[dmaphPcH]^0 in CHCl$_3$ (C – black, N – blue, H – white).

Figure S4. DFT optimized structure of ^{2}[dmaphPc]$^-$ in CHCl$_3$ (C – black, N – blue, H – white).

Figure S5. DFT calculated spin density of [4][dmaphPcAg][0] in CHCl$_3$ (0.001 a.u. isosurface).

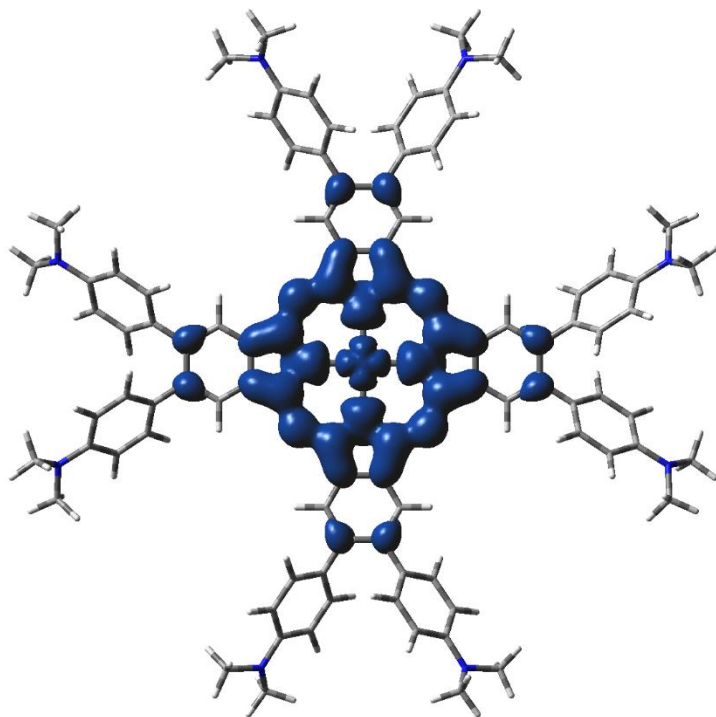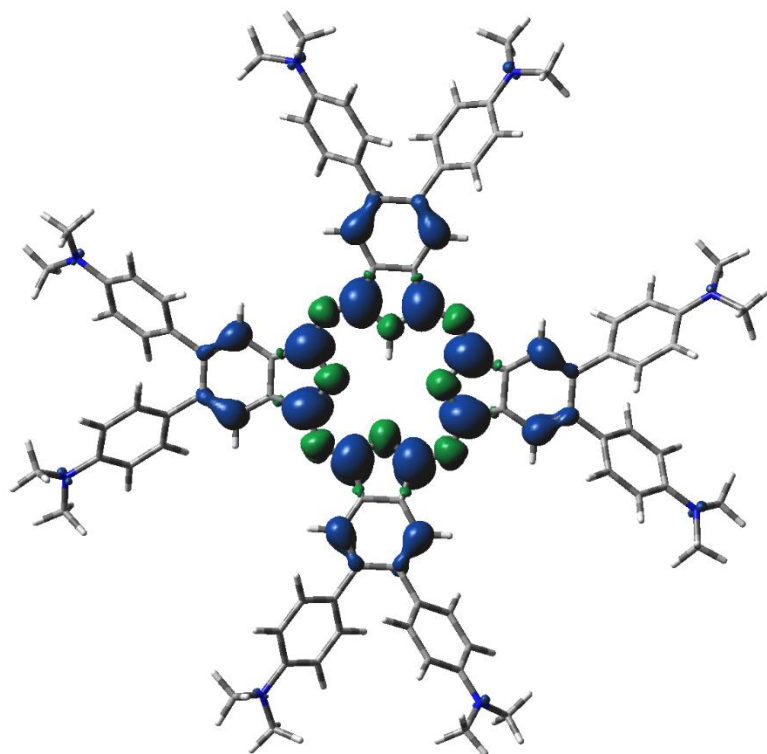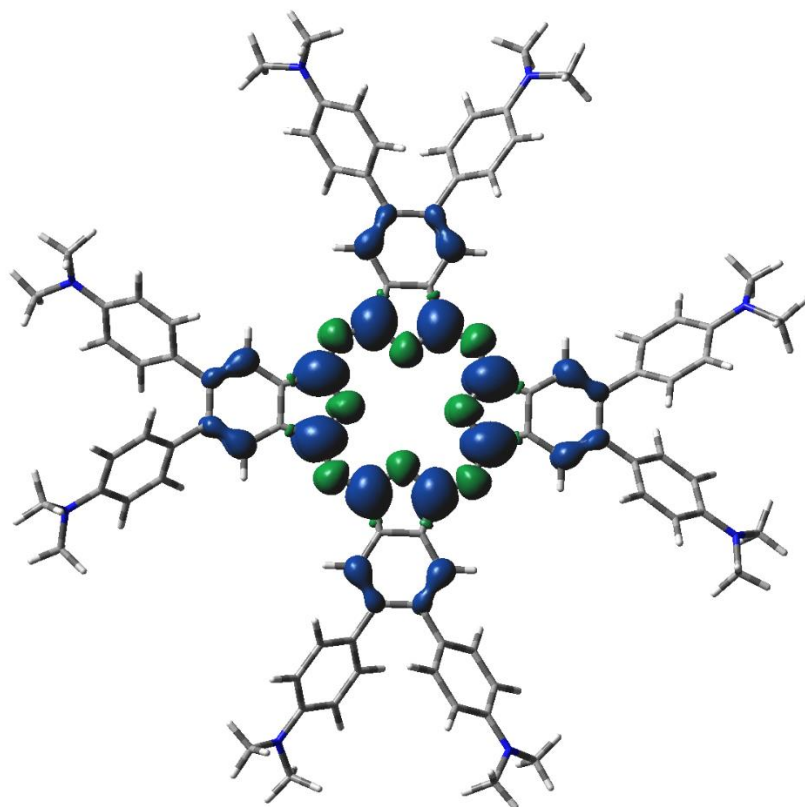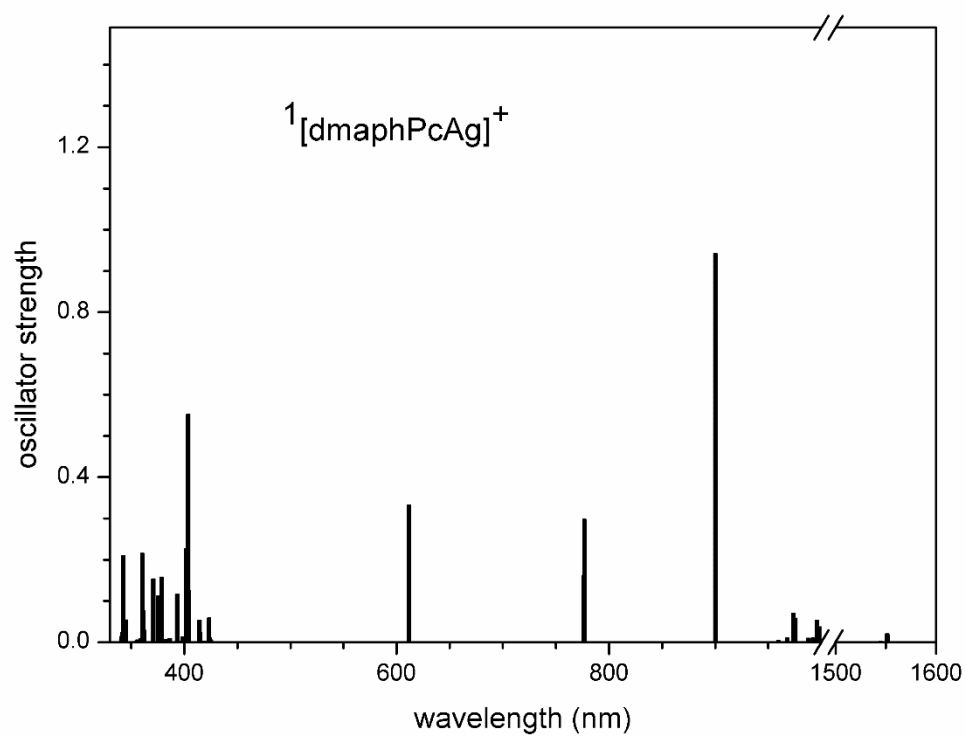Figure S6. DFT calculated spin density of [3][dmaphPcAg][-] in CHCl$_3$ (0.001 a.u. isosurface).

Figure S7. DFT calculated spin density of [4][dmaphPcAg][2-] in CHCl$_3$ (0.001 a.u. isosurface).

Figure S8. DFT calculated spin density of [2][dmaphPcH][0] in CHCl$_3$ (0.001 a.u. isosurface).

Figure S9. DFT calculated spin density of ^{2}[dmaphPc]$^-$ in CHCl$_3$ (0.001 a.u. isosurface).

Figure S10. TD-DFT calculated electron transitions in ^{1}[dmaphPcAg]$^+$ in CHCl$_3$.

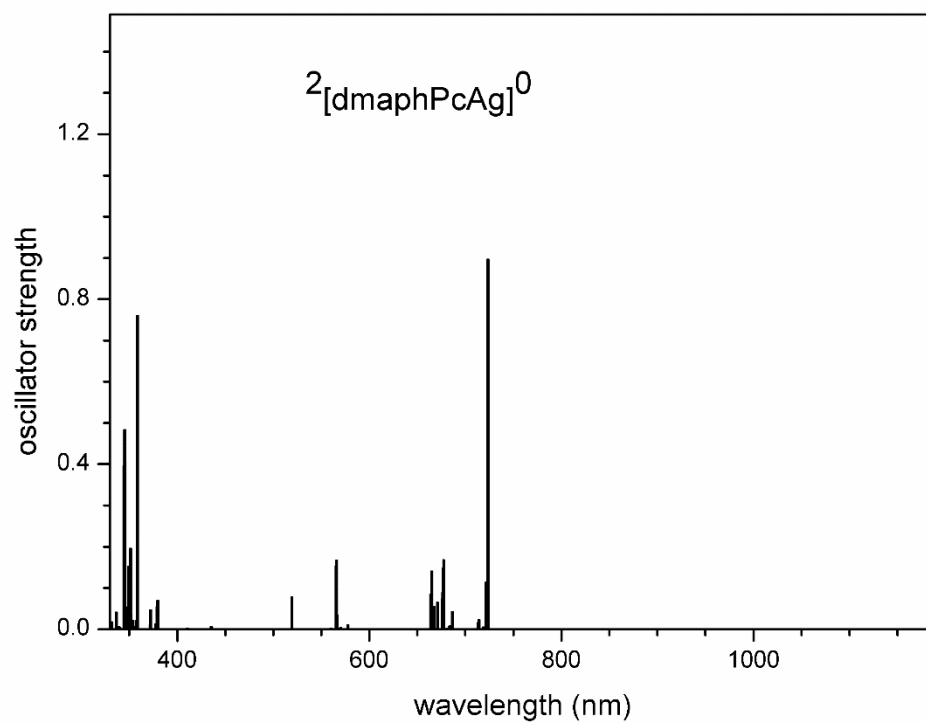Figure S11. TD-DFT calculated electron transitions in ^{3}[dmaphPcAg]$^+$ in CHCl$_3$.

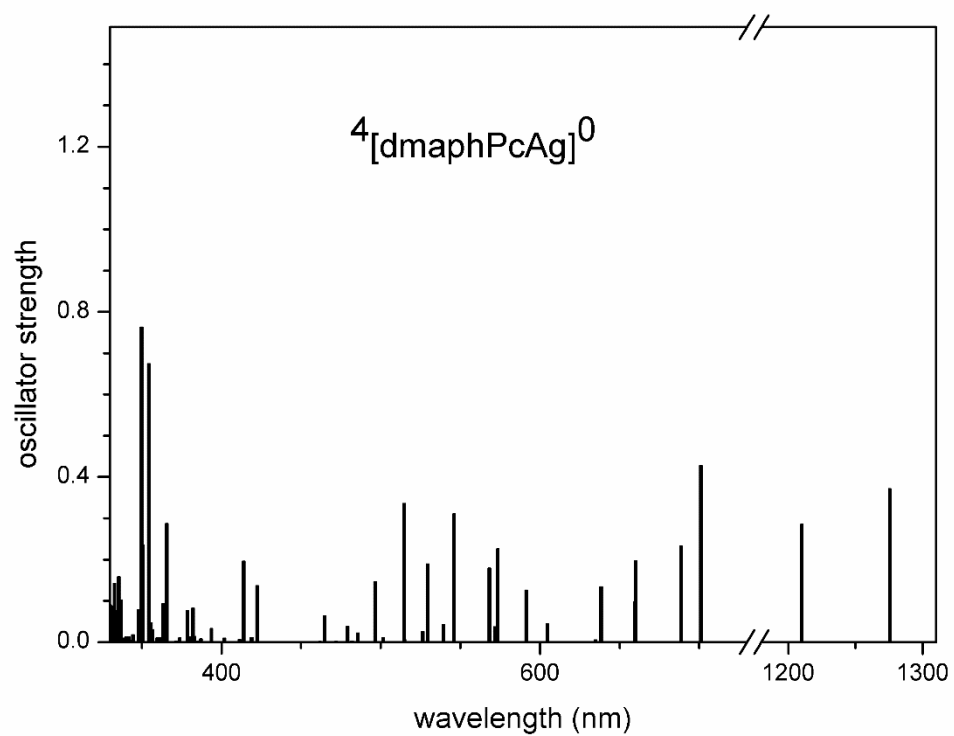Figure S12. TD-DFT calculated electron transitions in ^{2}[dmaphPcAg]^0 in CHCl$_3$.

Figure S13. TD-DFT calculated electron transitions in ^{4}[dmaphPcAg]^0 in CHCl$_3$.
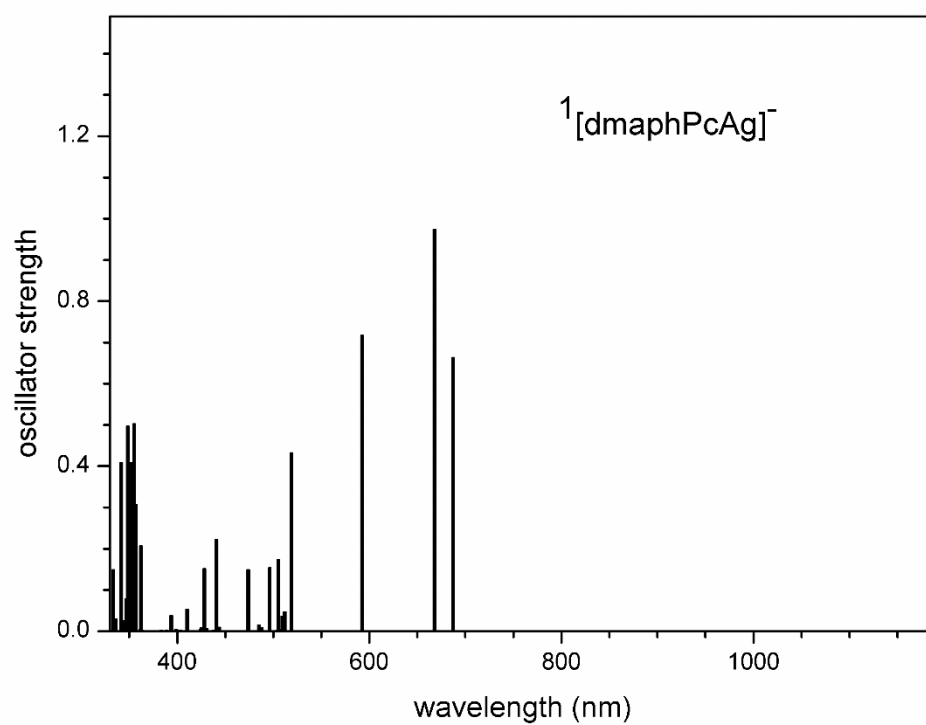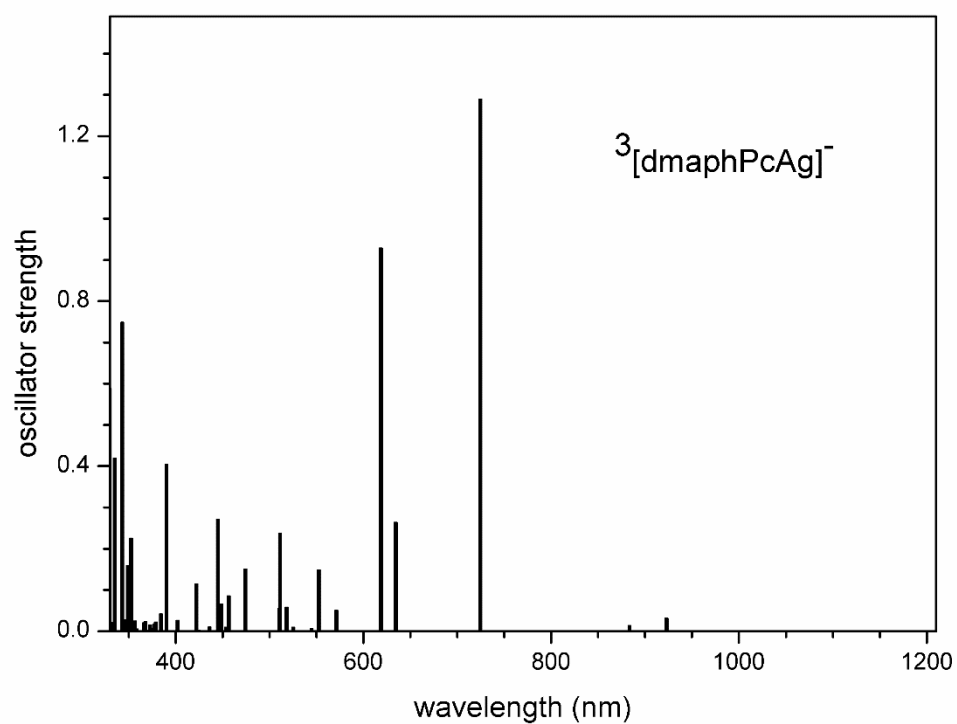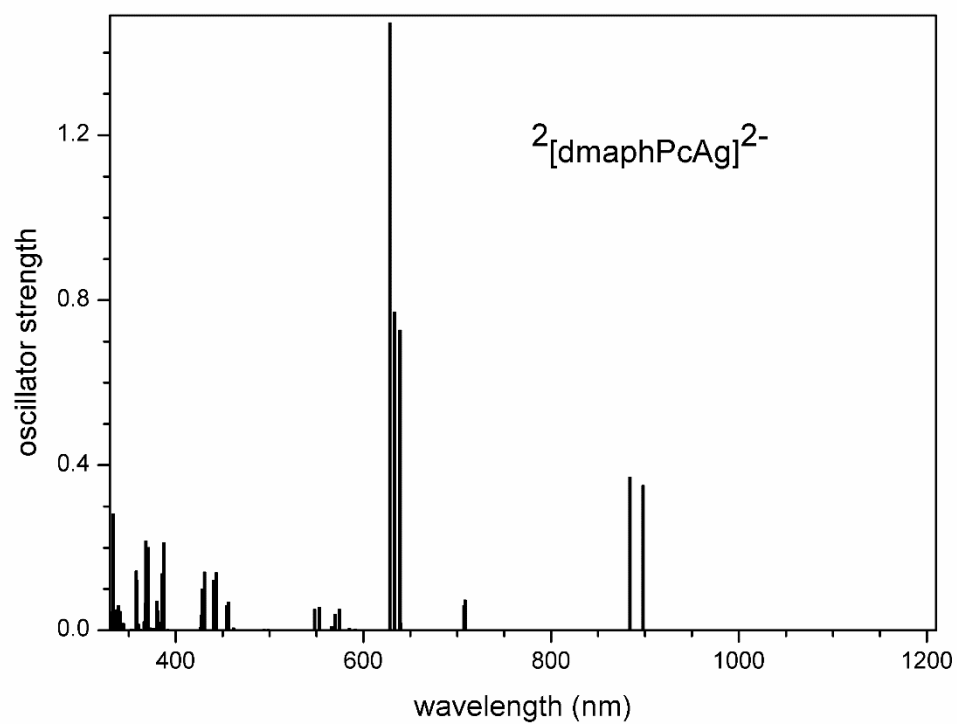

Figure S14. TD-DFT calculated electron transitions in ^{1}[dmaphPcAg]$^-$ in CHCl$_3$.

Figure S15. TD-DFT calculated electron transitions in ³[dmaphPcAg]⁻ in CHCl₃.

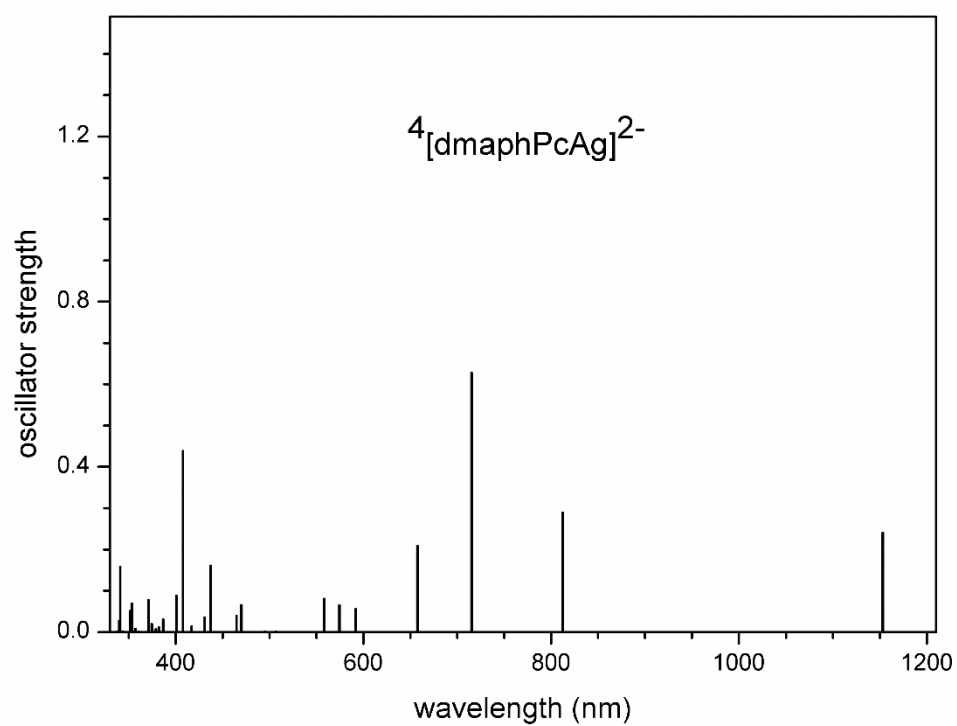Figure S16. TD-DFT calculated electron transitions in ²[dmaphPcAg]²⁻ in CHCl₃.

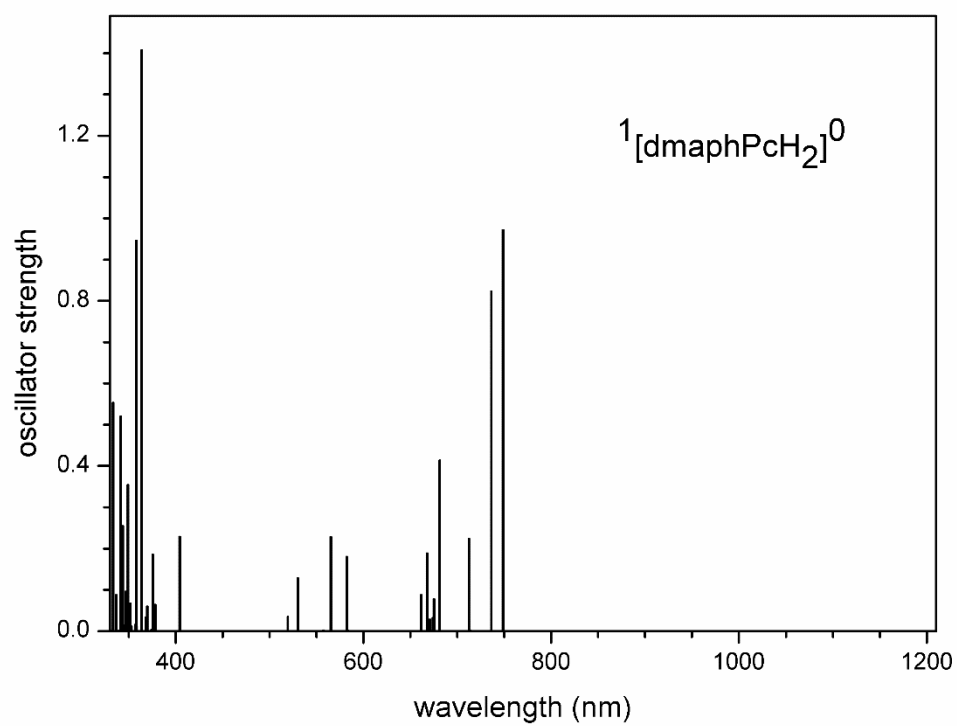Figure S17. TD-DFT calculated electron transitions in ^{4}[dmaphPcAg]$^{2-}$ in CHCl$_3$.

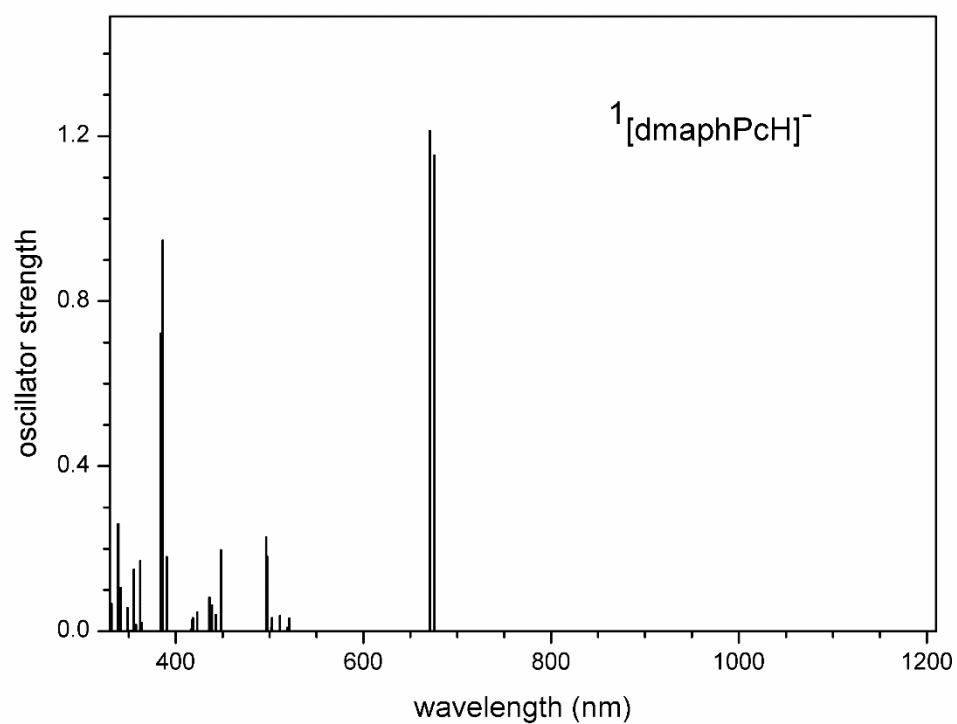Figure S18. TD-DFT calculated electron transitions in ^{1}[dmaphPcH$_2$]^0 in CHCl$_3$.

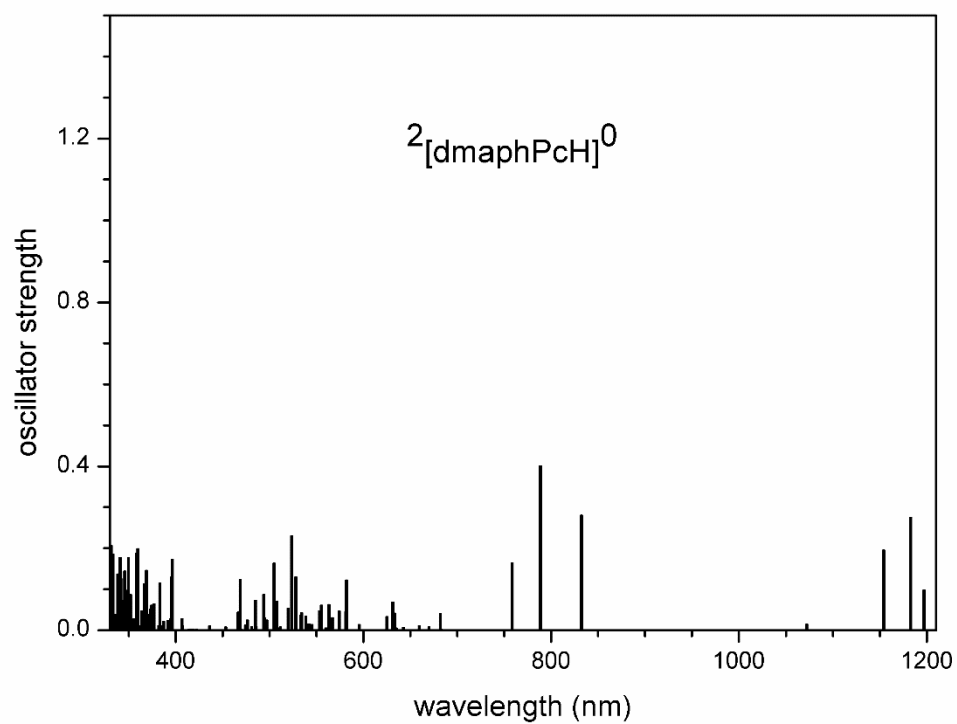Figure S19. TD-DFT calculated electron transitions in [1][dmaphPcH][-] in CHCl₃.

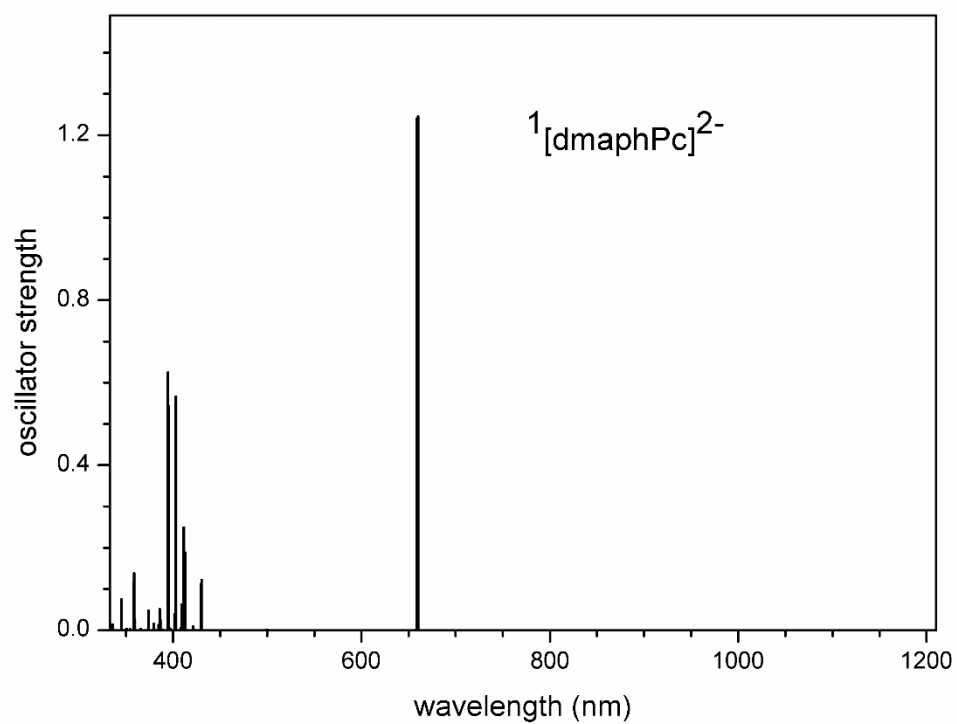Figure S20. TD-DFT calculated electron transitions in [2][dmaphPcH][0] in CHCl₃.

Figure S21. TD-DFT calculated electron transitions in ^{1}[dmaphPc]$^{2-}$ in CHCl$_3$.
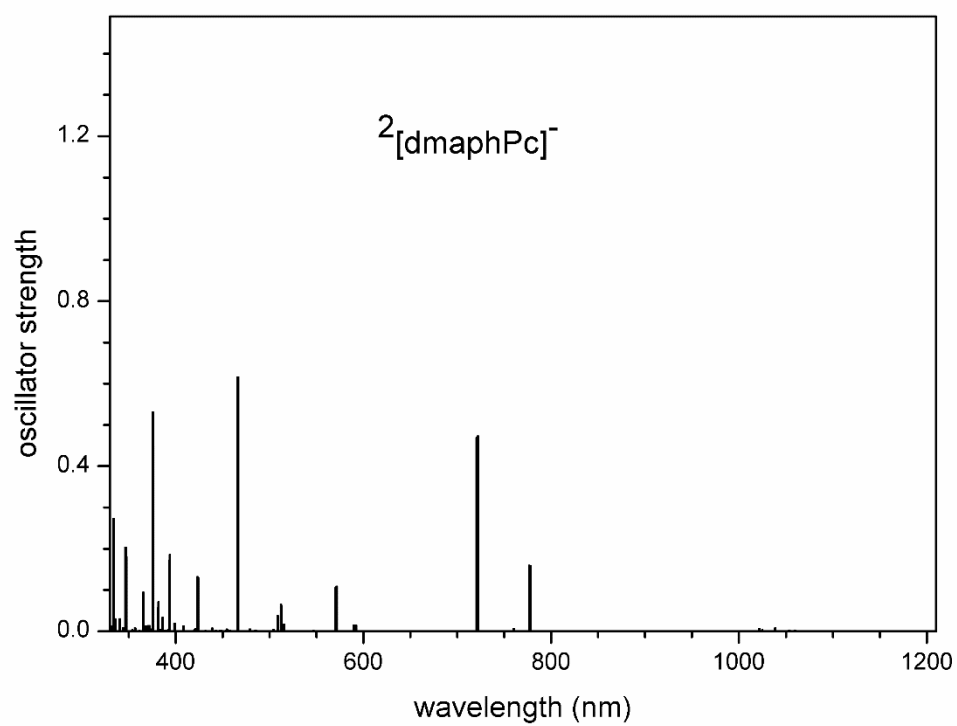

Figure S22. TD-DFT calculated electron transitions in ^{2}[dmaphPc]$^{-}$ in CHCl$_3$.

References

1. Breloy, L.; Alcay, Y.; Yilmaz, I.; Breza, M., Bourgon, J.; Brezová, V.; Yagci, Y., Versace, D.-L. Dimethyl amino phenyl substituted silver phthalocyanine as a UV- and visible-light absorbing photoinitiator: in situ preparation of silver/polymer nanocomposites. Polym. Chem. **2021**, 12, 1273-1285.