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

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Supplementary information

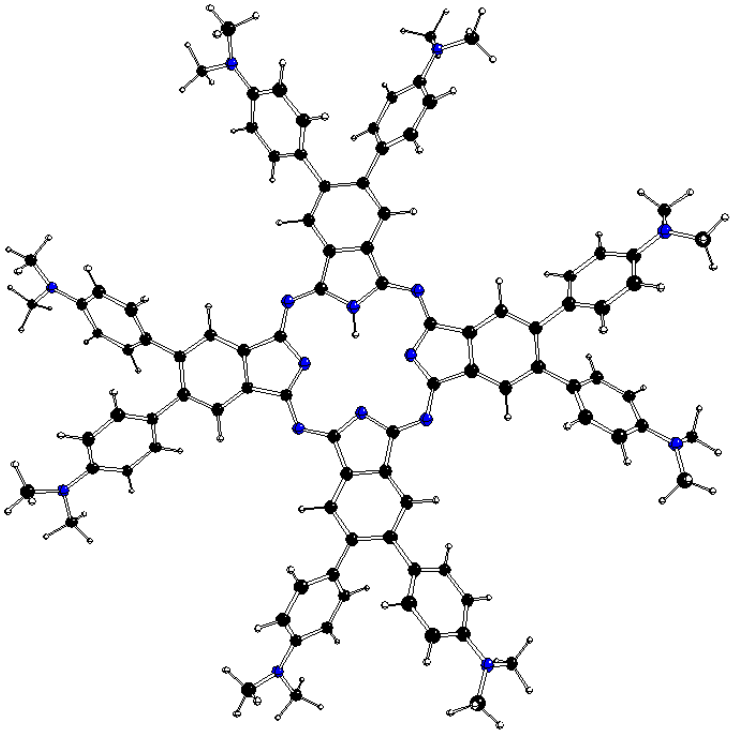

Figure S1. DFT optimized structure of $^{2}[dmaphPcH]^{0}$ in $CHCl_3$ (C – black, N – blue, H – white).

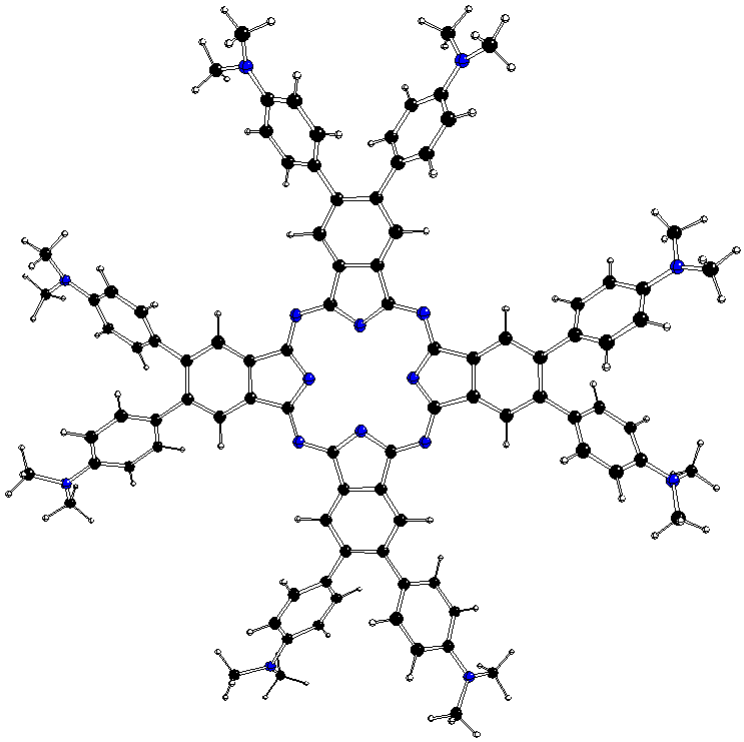

Figure S2. DFT optimized structure of $^{2}[dmaphPc]^{-}$ in $CHCl_3$ (C – black, N – blue, H – white).

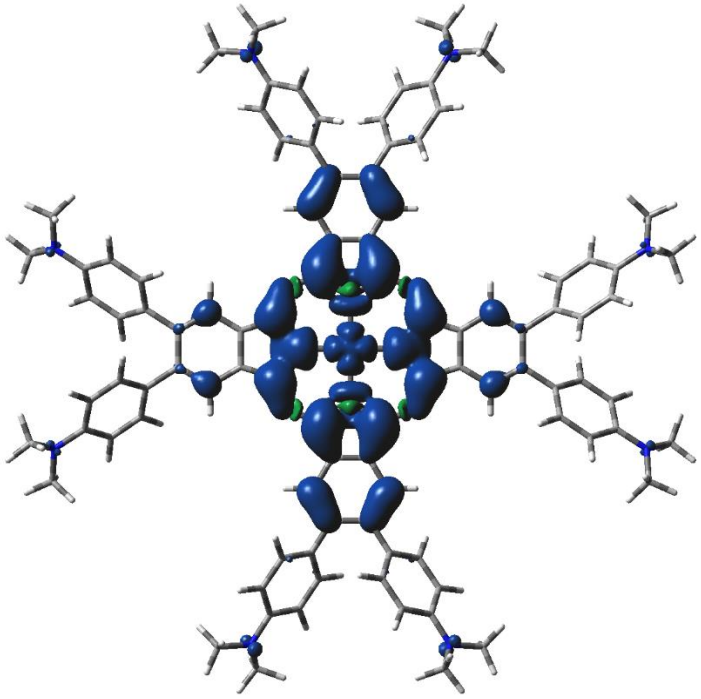

Figure S3. DFT calculated spin density of ^{4}[dmaphPcAg]^{0} in $CHCl_3$ (0.001 a.u. isosurface).

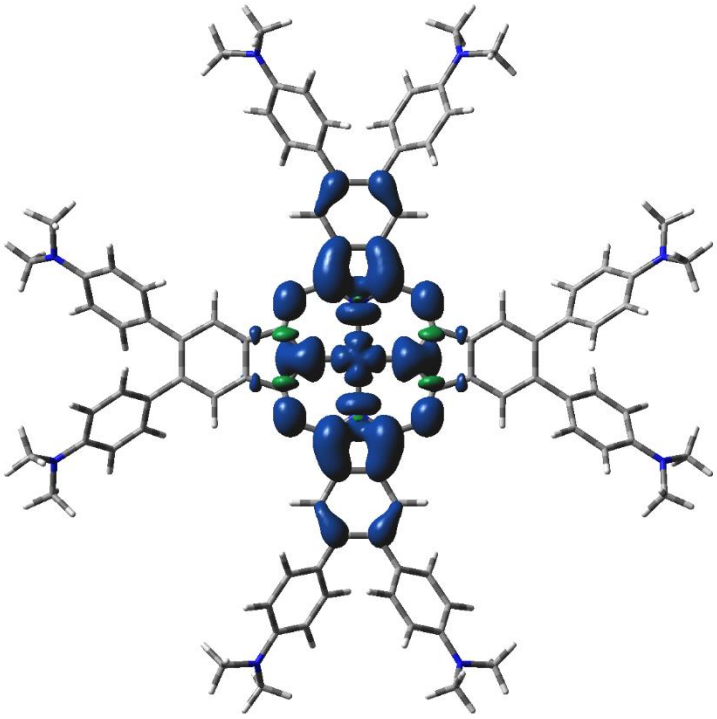

Figure S4. DFT calculated spin density of ^{3}[dmaphPcAg]$^{-}$ in $CHCl_3$ (0.001 a.u. isosurface).

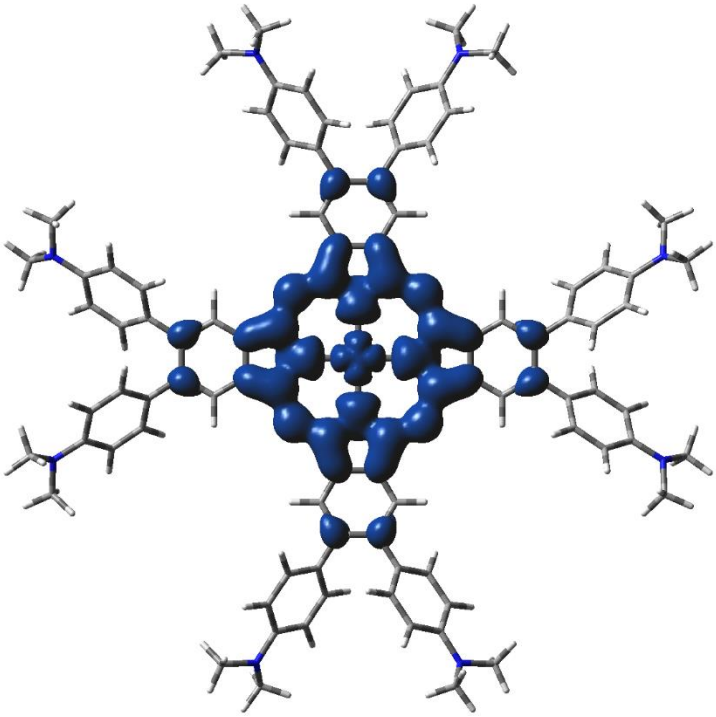

Figure S5. DFT calculated spin density of $^{4}[dmaphPcAg]^{2-}$ in $CHCl_3$ (0.001 a.u. isosurface).

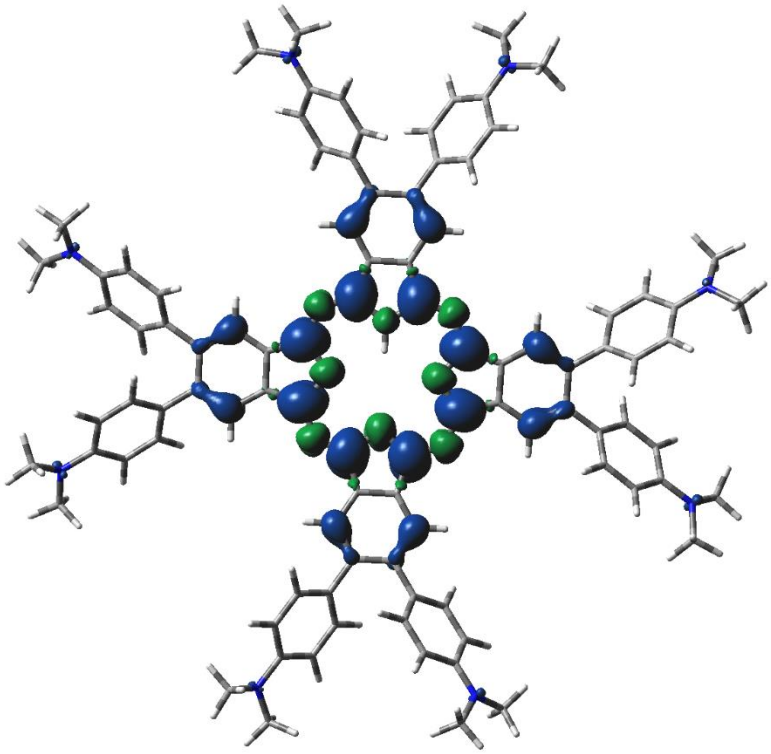

Figure S6. DFT calculated spin density of $^{2}[dmaphPcH]^{0}$ in $CHCl_3$ (0.001 a.u. isosurface).

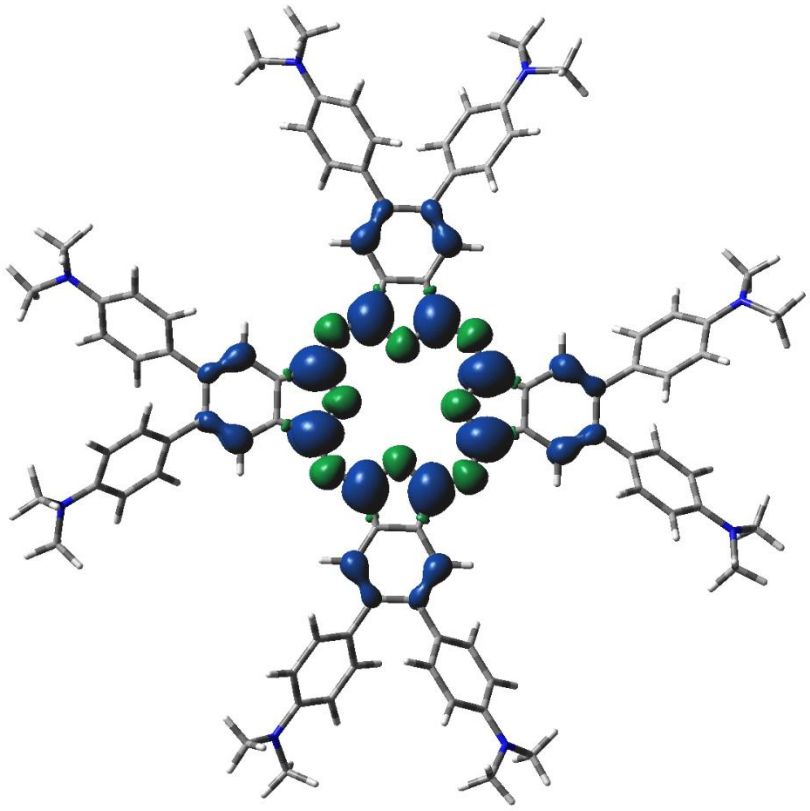

Figure S7. DFT calculated spin density of ^{2}[dmaphPc]$^{-}$ in $CHCl_3$ (0.001 a.u. isosurface).

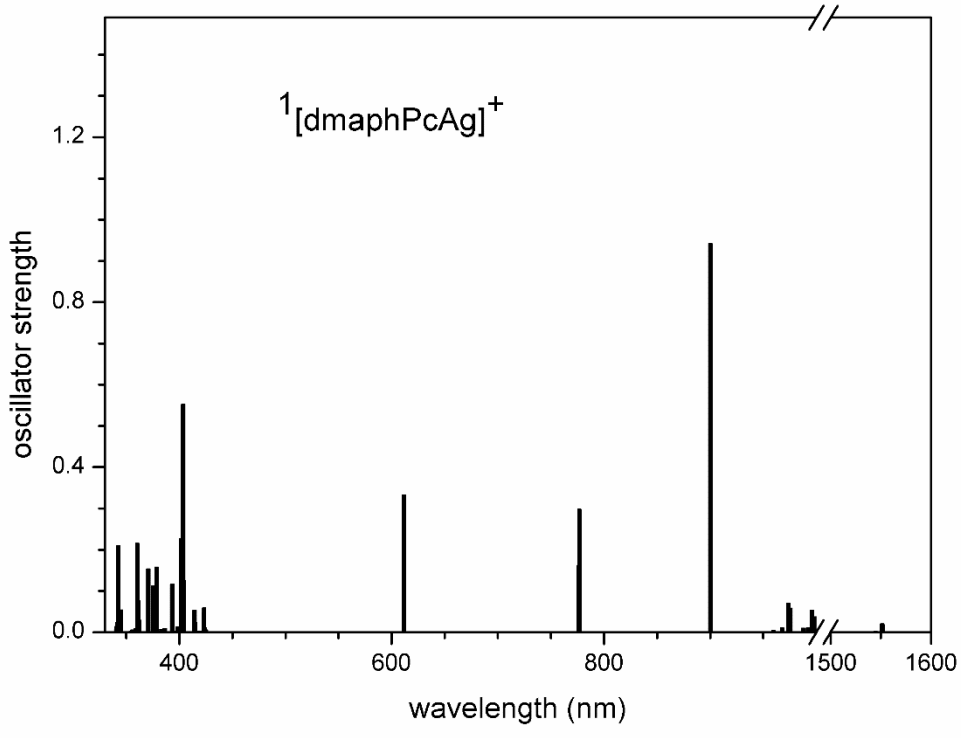

Figure S8. TD-DFT calculated electron transitions in ^{1}[dmaphPcAg]$^{+}$ in $CHCl_3$.

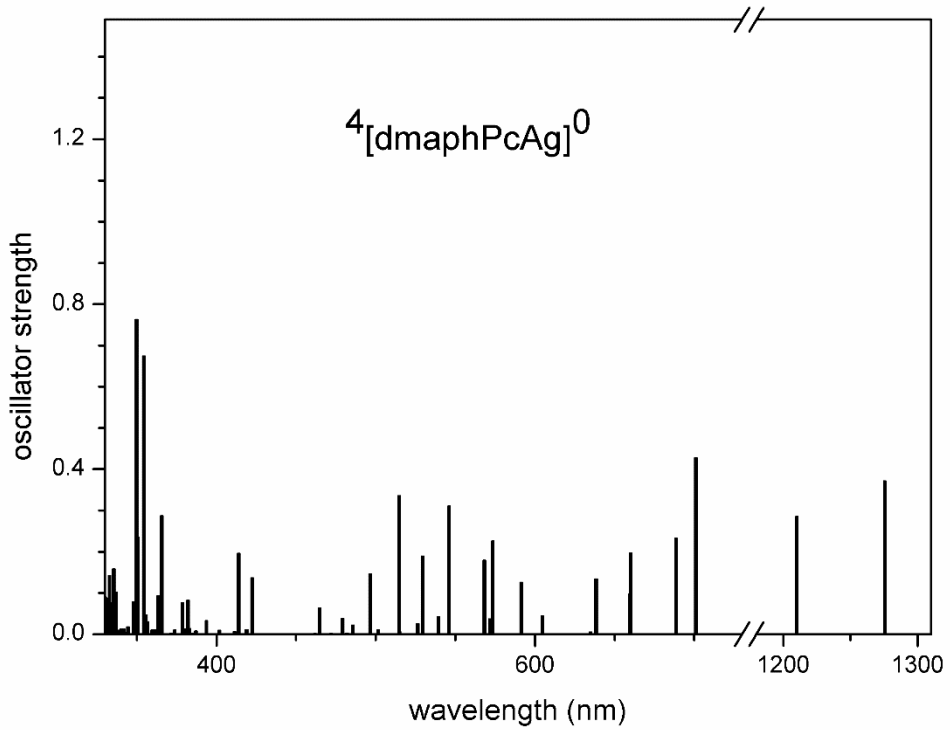

Figure S9. TD-DFT calculated electron transitions in ^{4}[dmaphPcAg]^0 in $CHCl_3$.

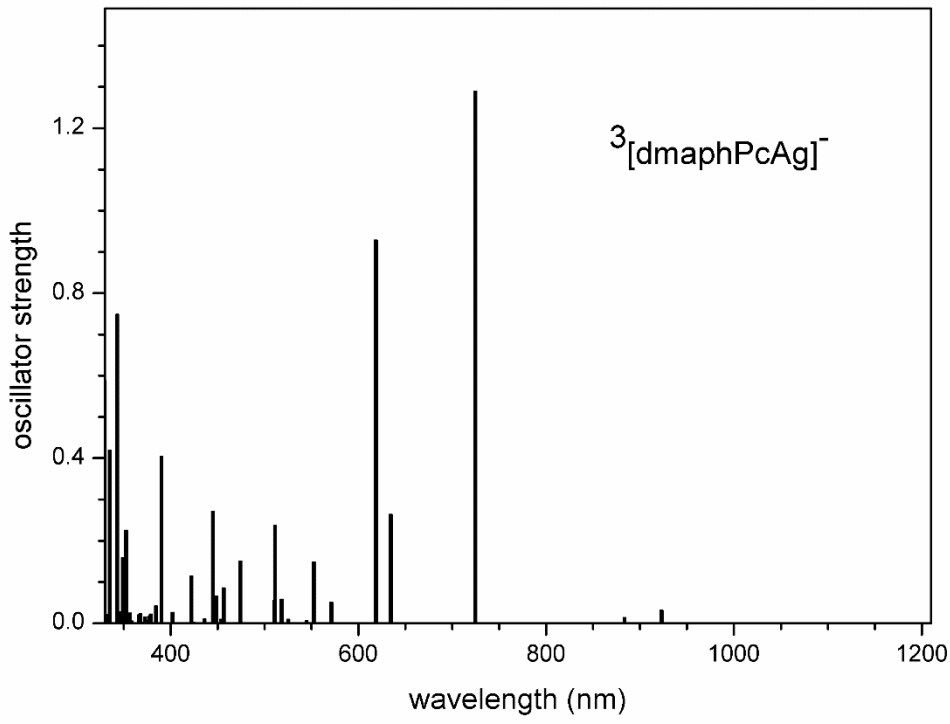

Figure S10. TD-DFT calculated electron transitions in ^{3}[dmaphPcAg]$^-$ in $CHCl_3$.

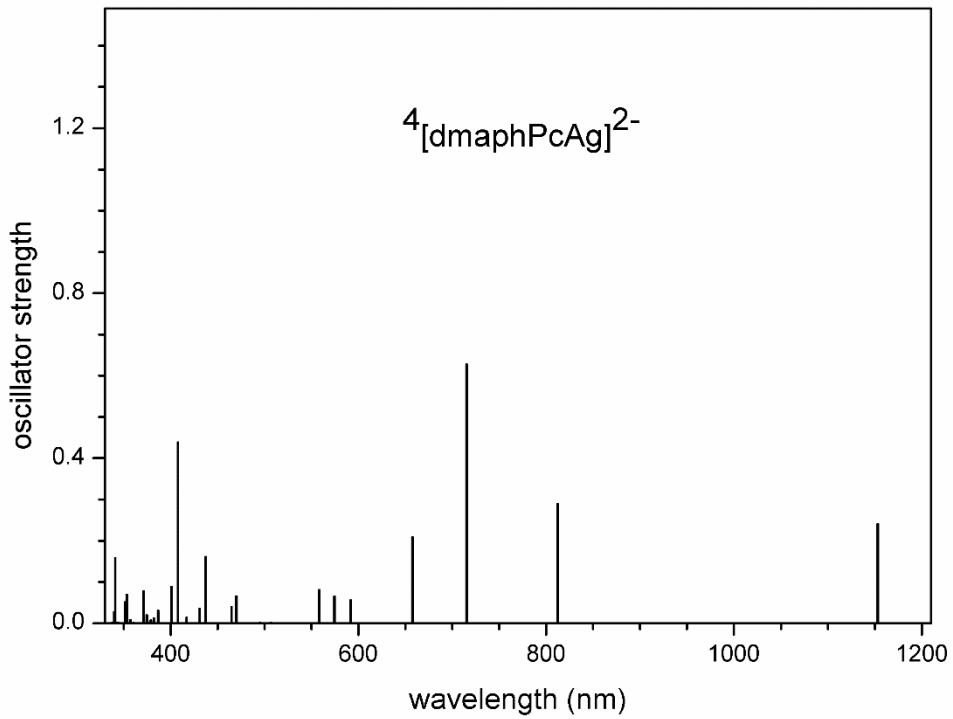

Figure S11. TD-DFT calculated electron transitions in ^{4}[dmaphPcAg]$^{2-}$ in $CHCl_3$.

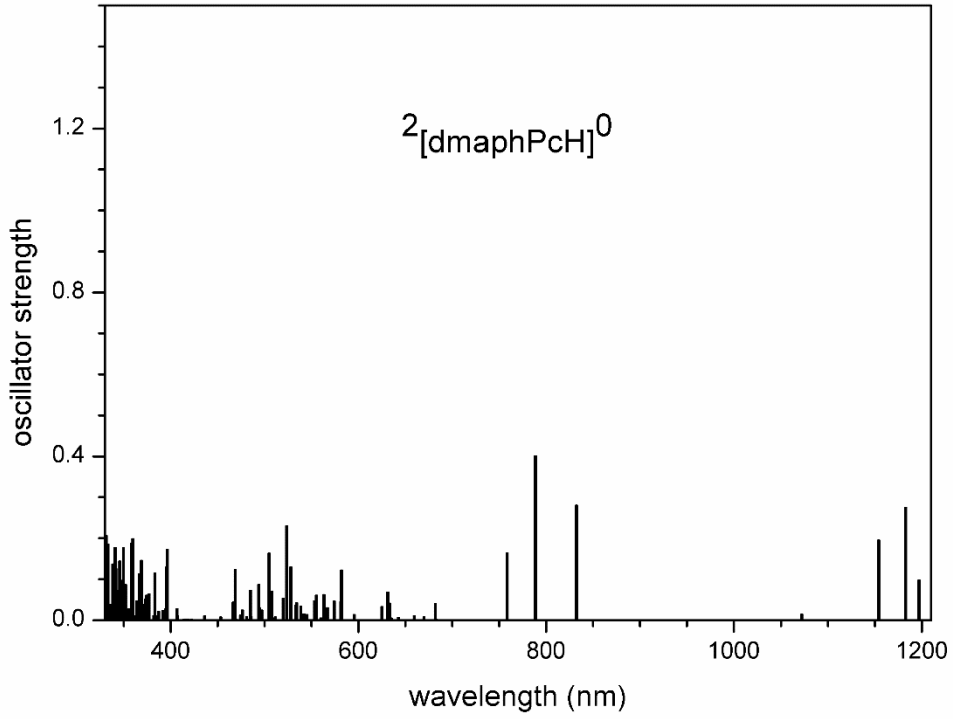

Figure S12. TD-DFT calculated electron transitions in ^{2}[dmaphPcH]^0 in $CHCl_3$.

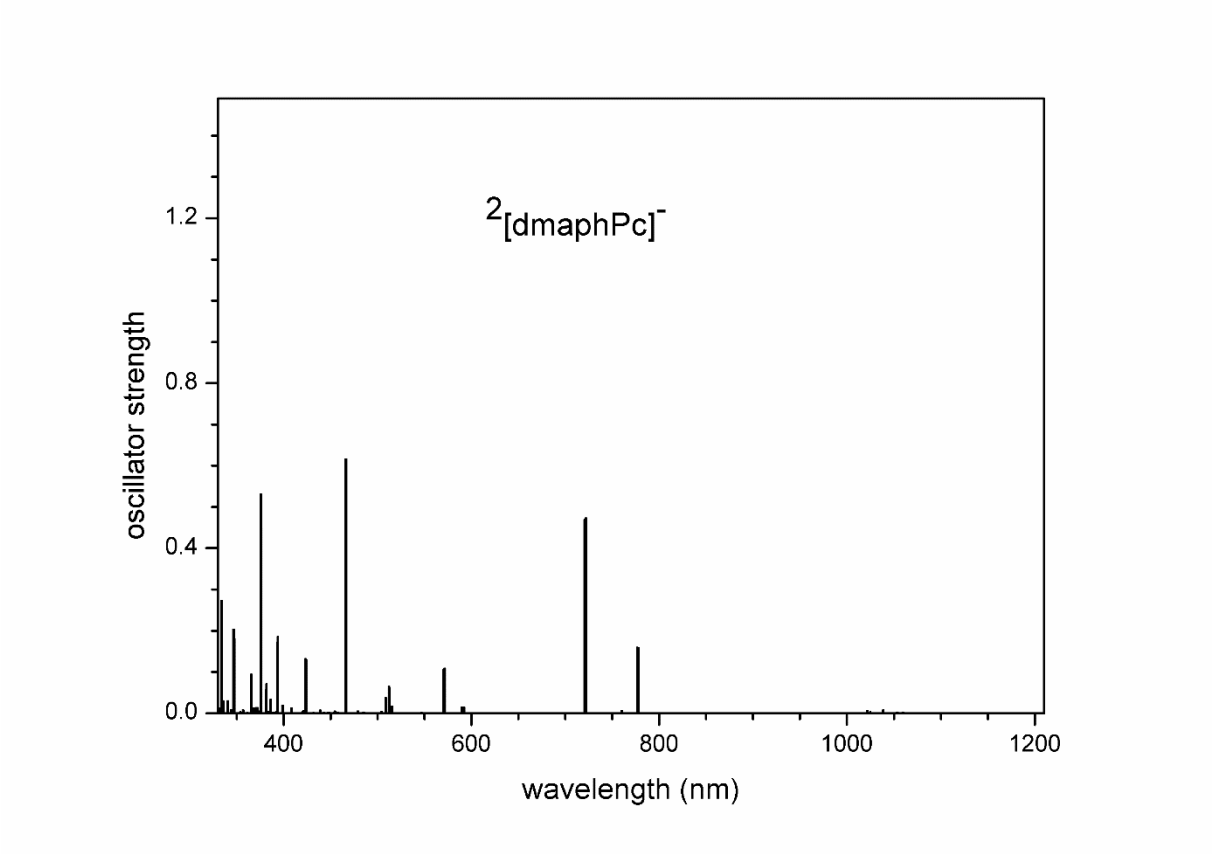

Figure S13. TD-DFT calculated electron transitions in ^{2}[dmaphPc]$^-$ in $CHCl_3$.