Supporting Information

Corrole-Fullerene Dyads: Formation of Long-Lived Charge-Separated States in Non-Polar Solvents

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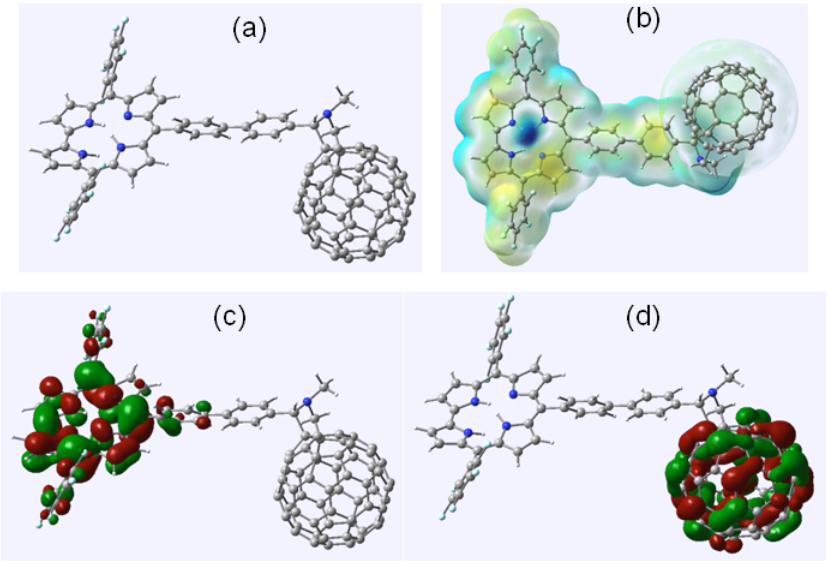

Figure S1. B3LYP/3-21G(*) calculated (a) optimized structure, (b) molecular electrostatic potential map, (c) frontier HOMO and (d) frontier LUMO of the corrole-fullerene dyad, **7**. The red and blue colors in (b) indicate the negative and positive electrostatic potentials.

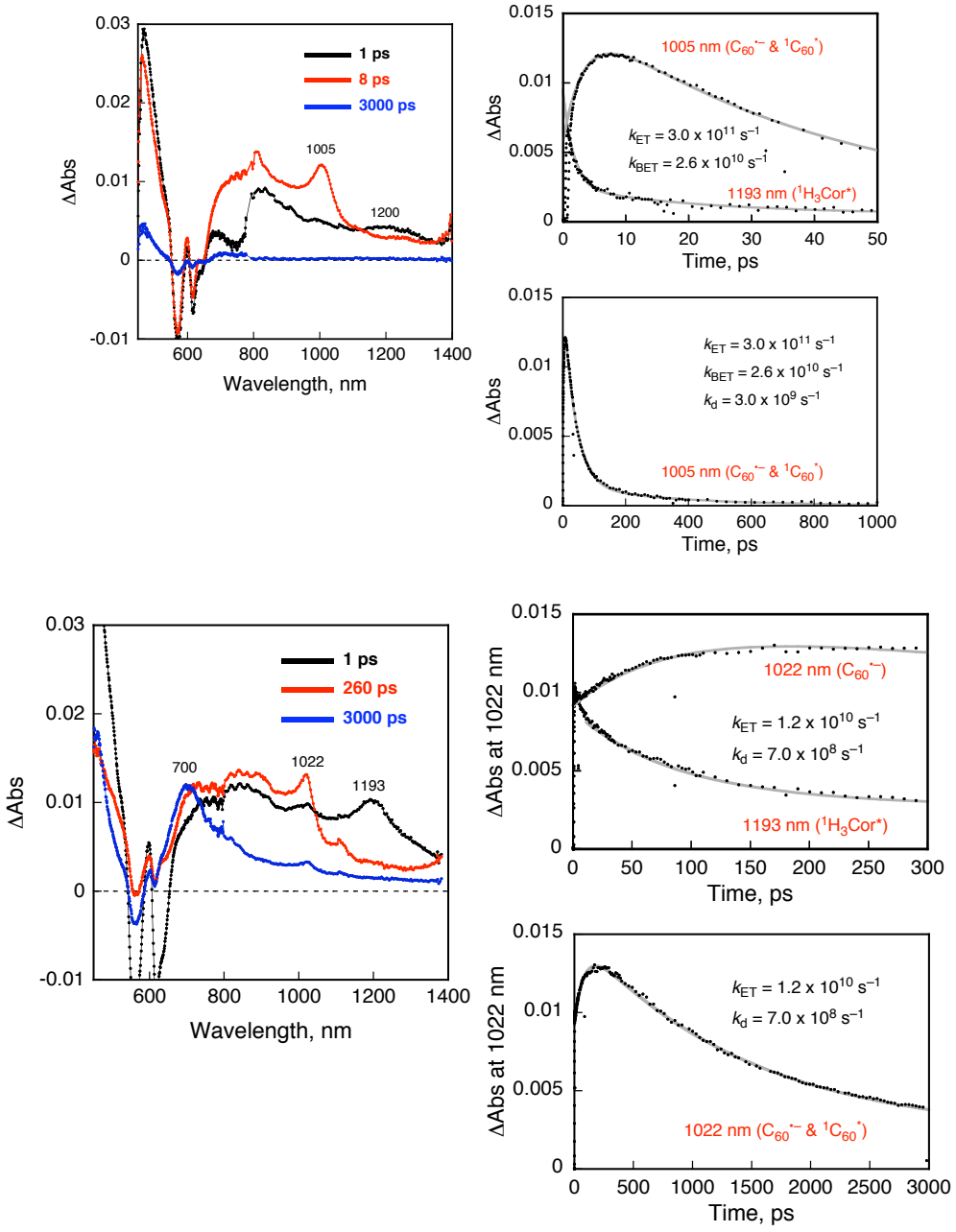

Figure S2. Femtosecond transient absorption spectra of the corrole-fullerene dyad, **6** in (a) THF and (b) cyclohexane.

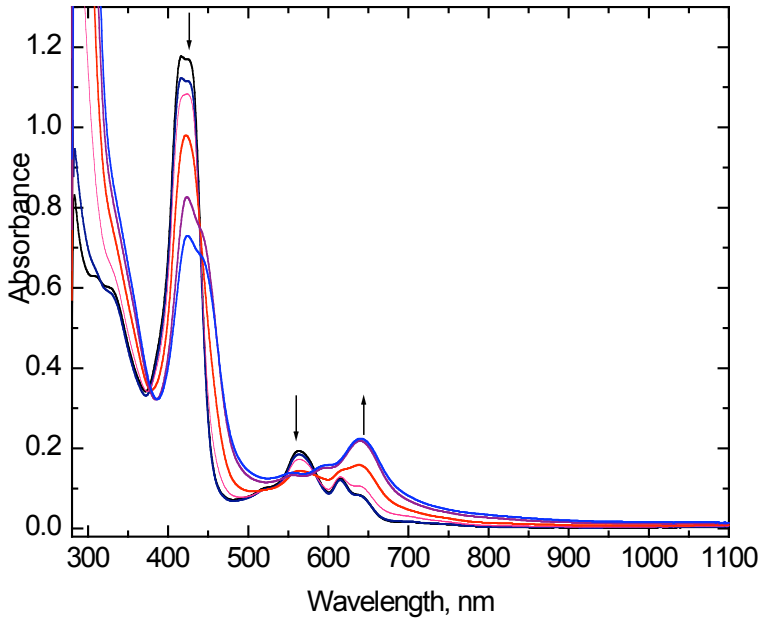

Figure S3. UV-visible spectra the corrole-fullerene dyad, **6** on increasing addition of nitronium hexafluoroantimonate (0.3 eq. each) oxidizing agent in toluene. The band at 640 nm is attributed to the formation of corrole π-cation radical.

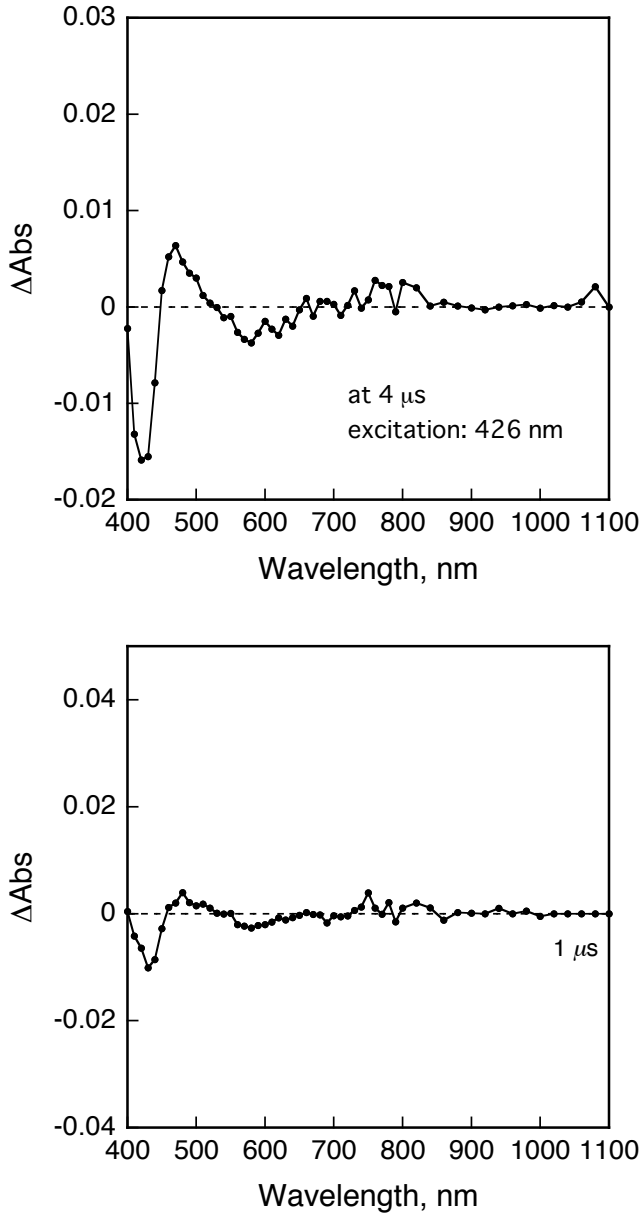

Figure S4. Nanosecond transient absorption spectrum (λ_{ex} = 532 nm) of the corrole-fullerene dyad, **6** in (a) benzonitrile and (b) THF.

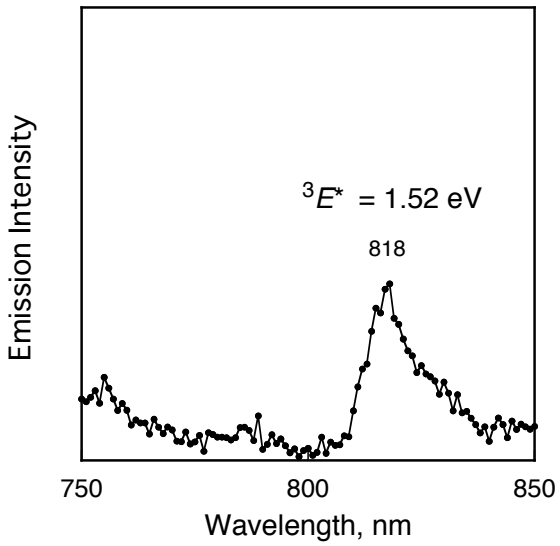

Figure S5. Phosphorescence spectrum of free-base corrole, **4** in 2-methyltetrahydrofuran glass at 77K.

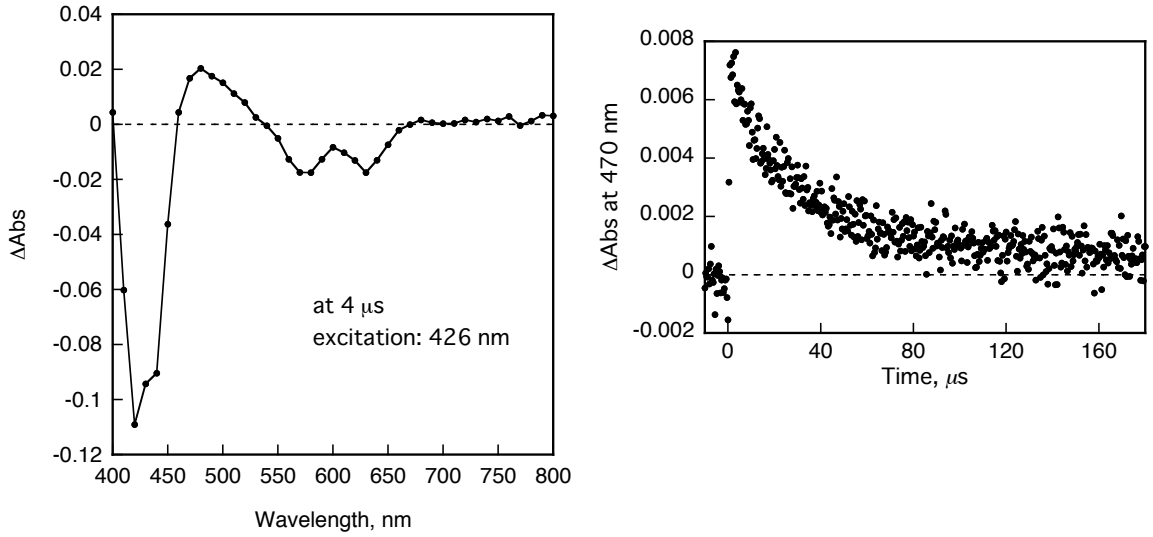

Figure S6. Nanosecond transient absorption spectrum (λ_{ex} = 532 nm) of free-base corrole, **4** in benzonitrile.

Gaussian 03, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J. A.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B. G.; Chen, W.; Wong, M. W.; Andres, J. L.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. Gaussian, Inc., Pittsburgh PA, 2003.