

Supporting Information

Sharing Orbitals – Ultrafast Excited State Deactivations with Different Outcome in Bucky Ferrocenes and Ruthenocenes

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Complete Ref. 25: Gaussian 98, Revision A.6, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, Jr., 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.; Chen, W.; Wong, M. W.; Andres, J. L.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. Gaussian Inc., Pittsburgh PA, 1998.

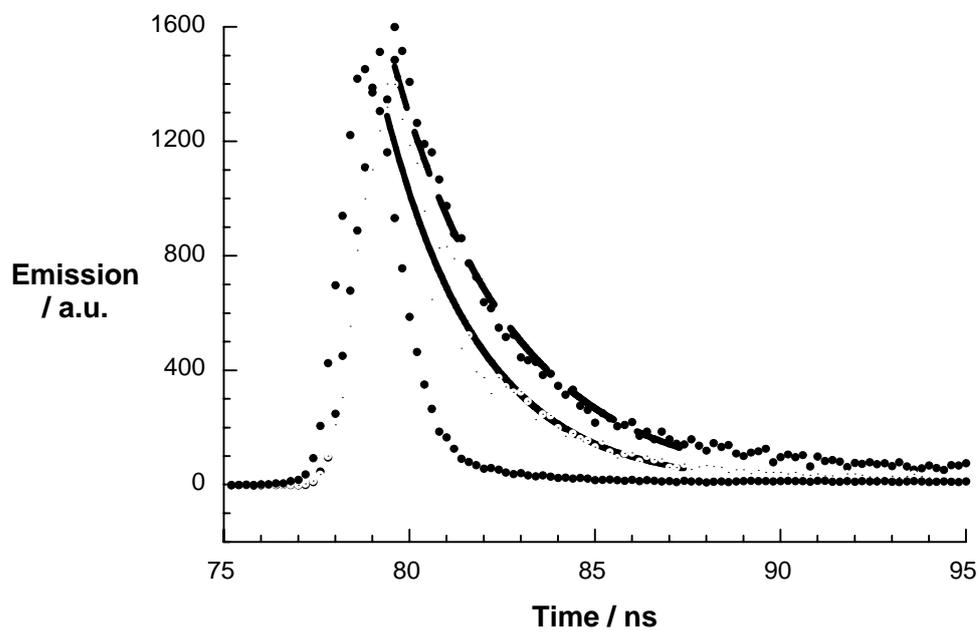


Figure S1: Time-resolved fluorescence profiles at 620 nm illustrating the fluorescence lifetimes of C₆₀Me₅H (dashed line), Ru(C₆₀Me₅)Cp (solid line) and laser scatterer recorded upon 337 nm laser excitation.

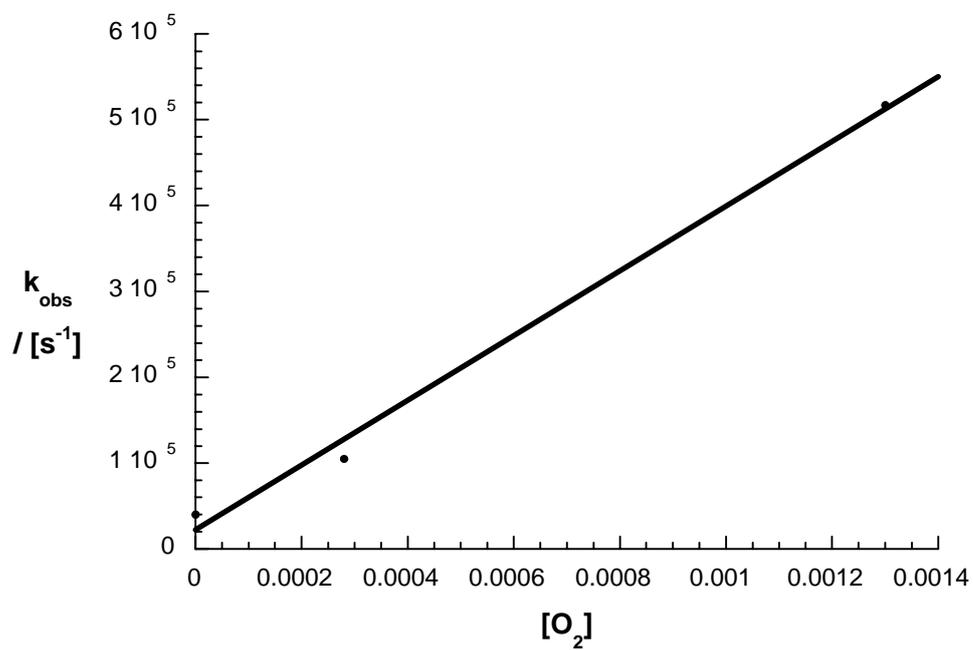


Figure S2: Plot of k_{obs} vs $[\text{O}_2]$ monitored at 660 nm for the energy transfer process from triplet excited $\text{C}_{60}\text{Me}_5\text{H}$ to molecular oxygen.

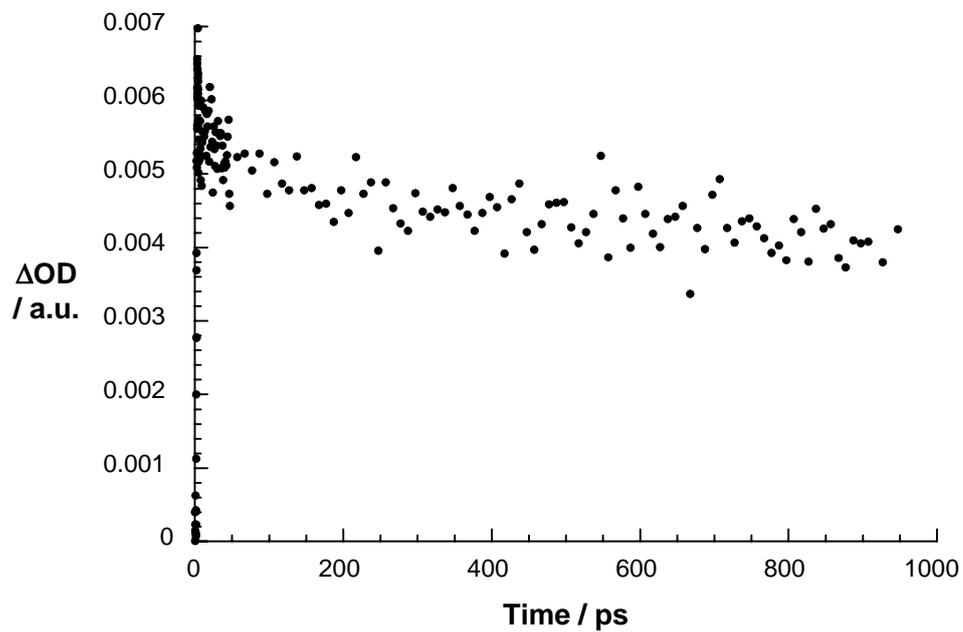


Figure S3: Time-absorption profiles at 650 nm recorded upon femtosecond flash photolysis (387 nm) of Ru(C₆₀Ph₅)Cp in nitrogen saturated toluene solution, monitoring the decay of the fullerene singlet excited state.

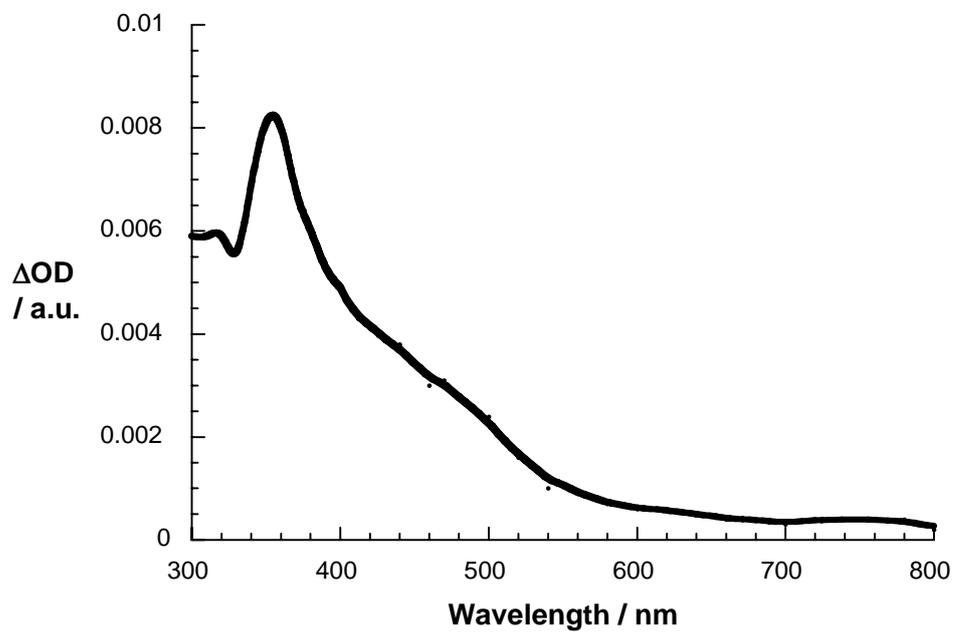


Figure S4: Differential absorption spectrum (visible) obtained upon pulse radiolytic oxidation of $\text{Ru}(\text{Cp})_2$ in aerated dichloromethane.