Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Modulating the $M_2\delta$-to-Ligand Charge Transfer Transition by the use of Diarylboron Substituents

Samantha E. Brown-Xu, Malcolm H. Chisholm*, Christopher B. Durr, Thomas F. Spilker, and Philip J. Young

Department of Chemistry and Biochemistry, The Ohio State University, 100 West 18th Avenue, Columbus, Ohio 43210-1185

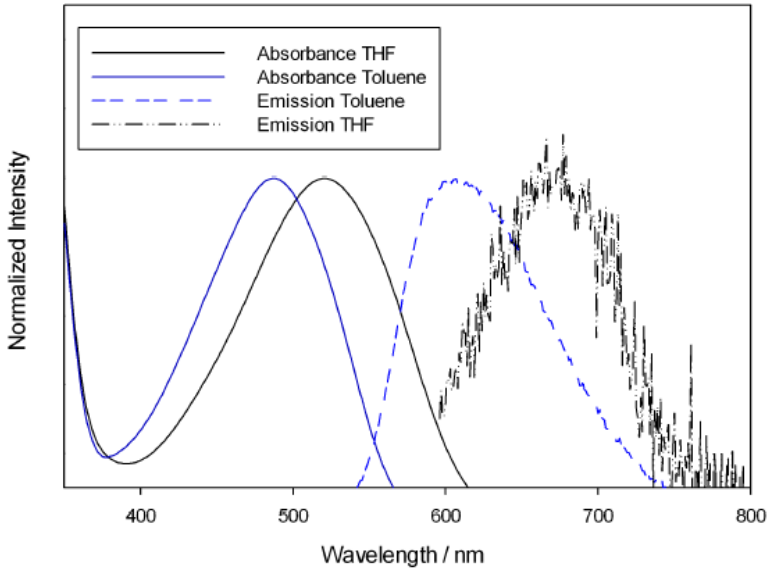

Fig S1. The electronic absorption and emission spectra of **I** in toluene and THF.

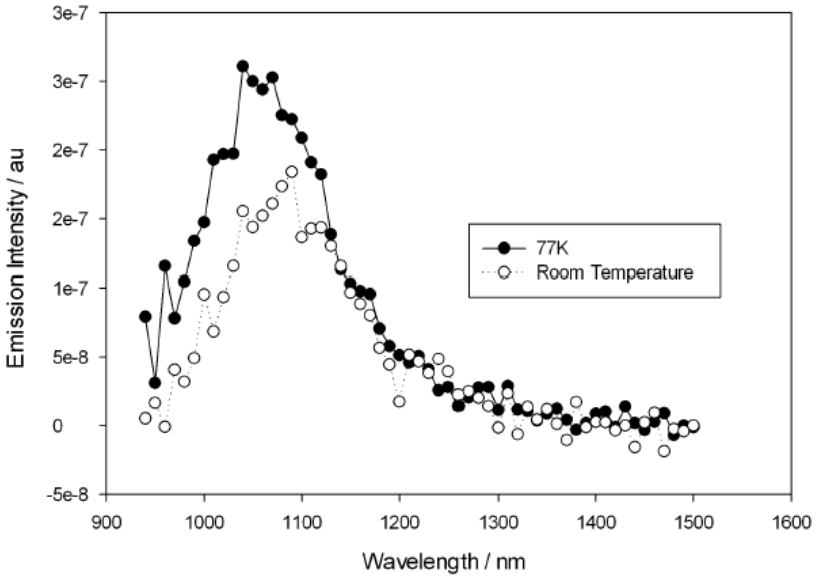

Fig S2. The phosphorescence spectra of **I** at RT and 77 K, λ_{ex} = 405.

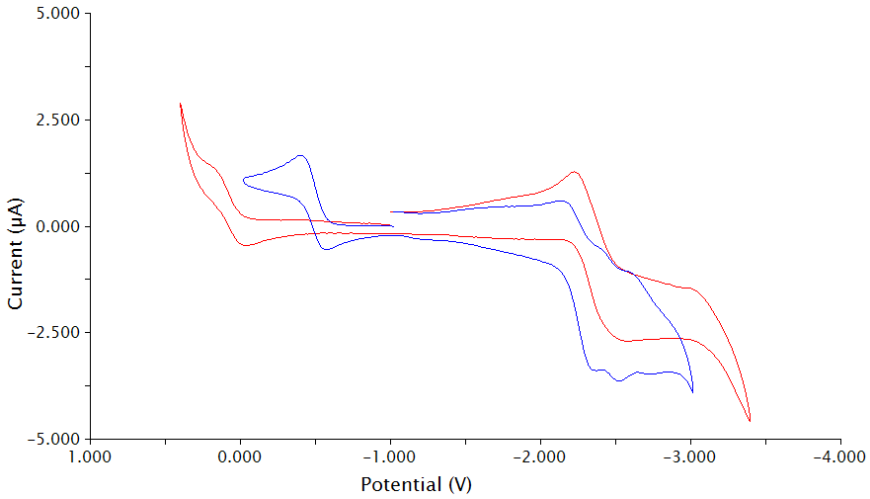

Fig S3. Cyclic voltammogram of compounds **I** and **II** in THF.

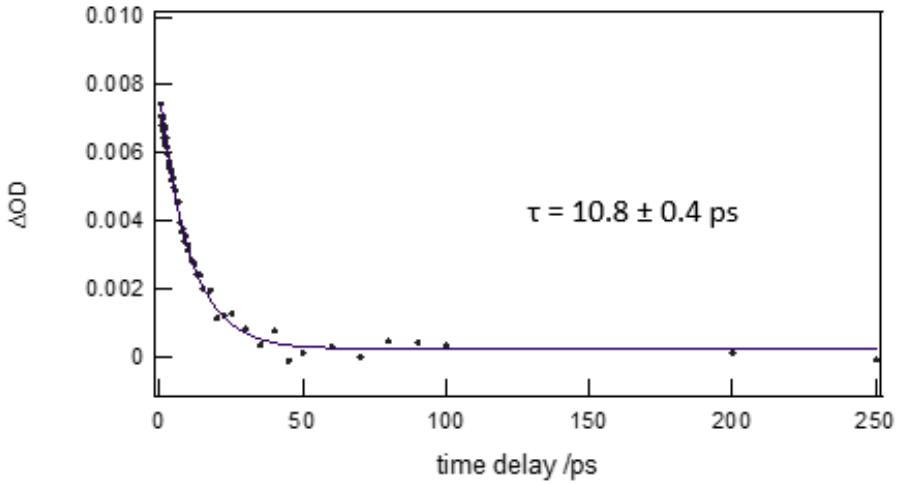

Fig S4. Kinetic trace from fsTA spectra of **I** in THF monitored at 390 nm.

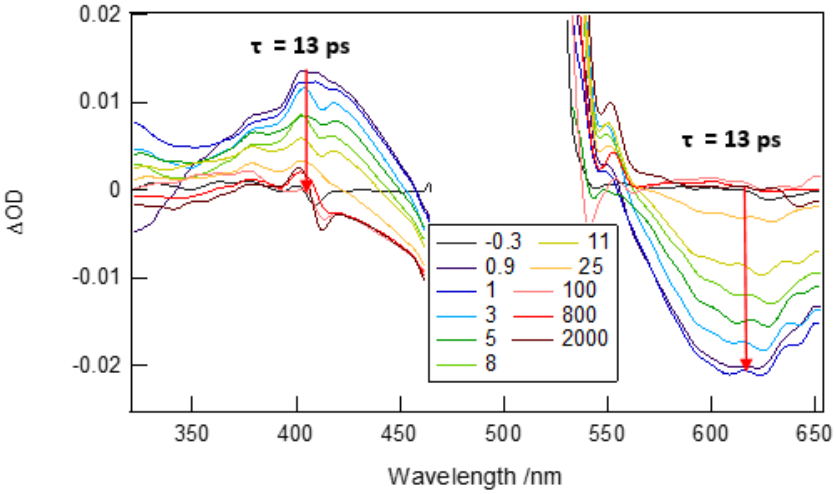

Fig S5. fs-TA spectrum of **I** in toluene at RT, λ_{ex} = 568 nm.

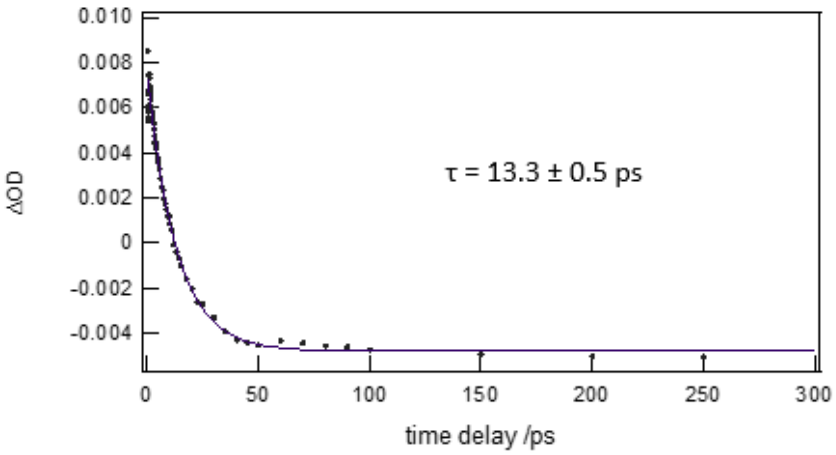

Fig S6. Kinetic trace from fsTA spectra of **I** in toluene monitored at 419 nm.

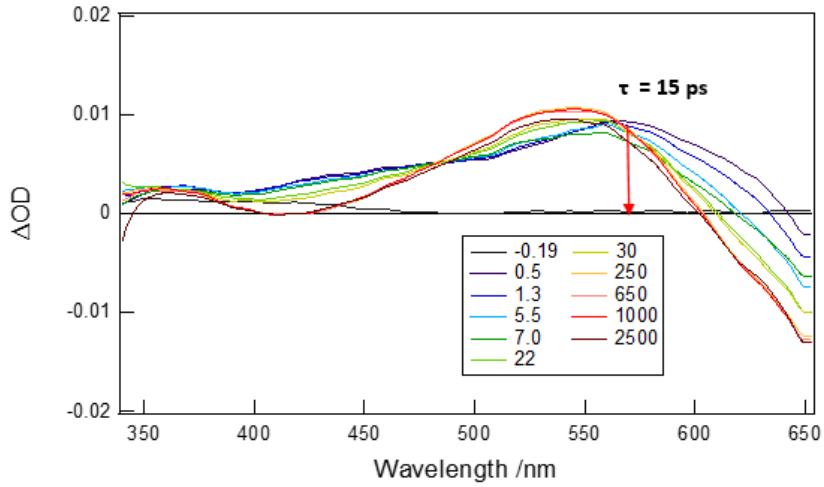

Fig S7. fs-TA spectrum of **II** in THF at RT, λ_{ex} = 800 nm.

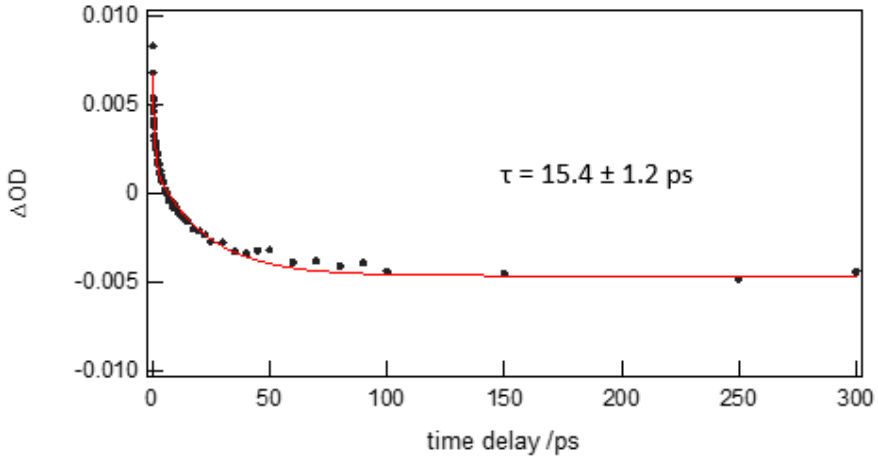

Fig S8. Kinetic trace from fsTA spectra of **II** monitored at 620 nm.

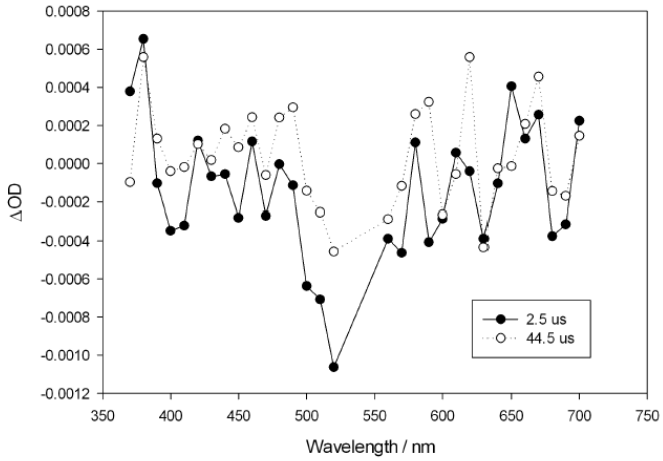

Fig S9. ns-TA spectrum of **I** in THF at RT, λ_{ex} = 532 nm.

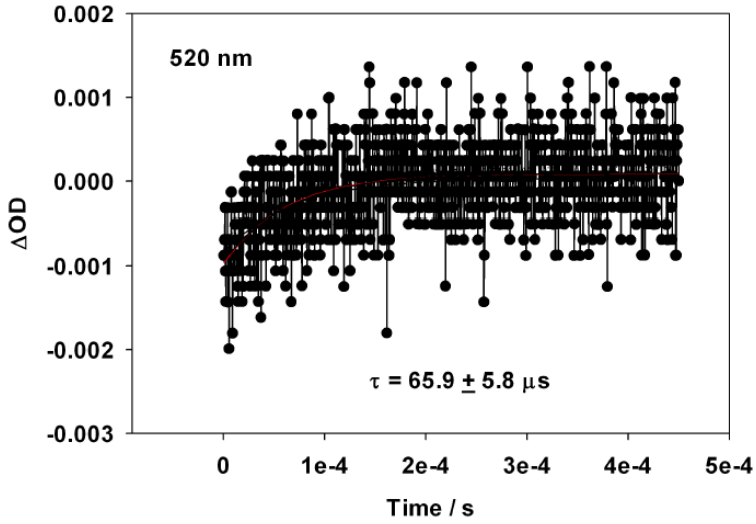

Fig S10. Kinetic trace from nsTA spectra of **I** monitored at 520 nm.

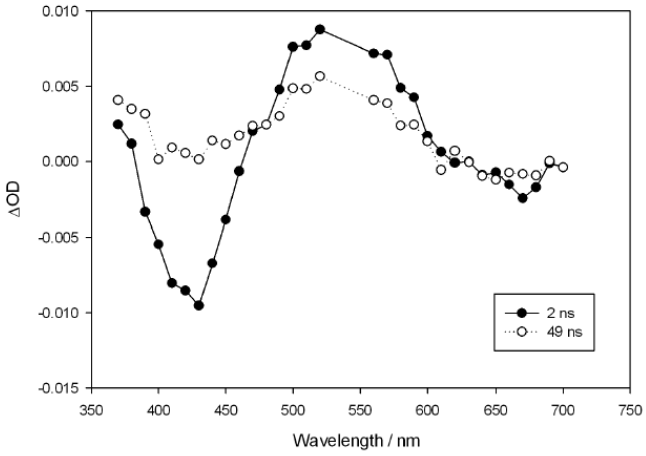

Fig S11. ns-TA spectrum of **II** in THF at RT, λ_{ex} = 355 nm.

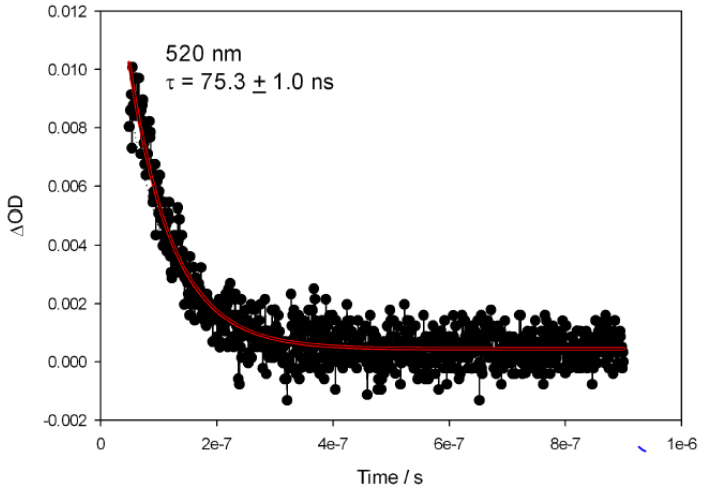

Fig S12. Kinetic trace from nsTA spectra of **II** monitored at 520 nm.

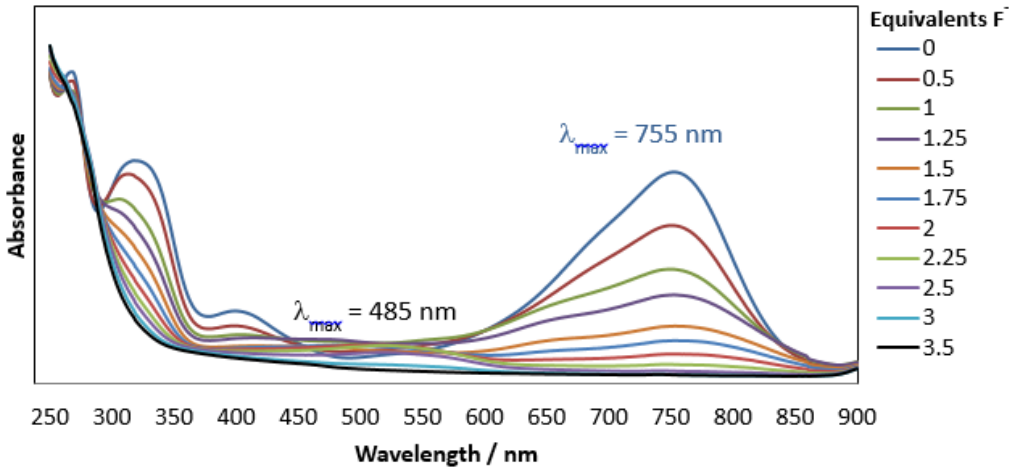

Fig S13. Absorption spectrum of **II** in THF titrated with fluoride ions. The compound decomposes upon the addition of water and could not be regenerated.

Table S1. Crystallographic supporting information.

Compound	$Mo_2(T^iPB)_2(Bz)_2$
Chemical formula	$C_{54}H_{72}Mo_2O_{10}$
Formula weight	1072.99
Temperature (K)	150(2)
Space group	Triclinic, P-1
a (Å)	10.2136(2)
b (Å)	10.3526(2)
c (Å)	12.6092(2)
α (°)	83.0670(10)
B (°)	80.8170(10)
γ (°)	84.8880(10)
V ($Å^3$)	1303.23(4)
Z	1
D_{calcd} (Mg/m^3)	1.367
Crystal Size (mm)	0.31 X 0.15 X 0.12
Theta range for data collection	0.74 to 27.49°
μ,(Mo, Kα) (mm^{-1})	0.536
F(000)	560
Reflections collected	38070
Unique reflections	5984 [R(int)= 0.059]
Completeness to θ_{max}	99.7%
Data/restraints/parameters	5984 / 103 / 462
R1[a] (%) (all data)	4.26 (7.75)
wR2[b](%)(all data)	10.05 (13.63)
Goodness-of-fit on F^2	1.119
Largest diff. peak and hole (e $Å^{-3}$)	0.647 and -1.192

[a]R1 = Σ | |F_o|-|F_c| | / Σ |F_o| X 100

[b]wR2 = { Σ [*w*(F_o^2-F_c^2)^2] / Σ [*w*(F_o^2)^2] }$^{1/2}$ X 100