Supporting Information

Molybdenum-Molybdenum Quadruple Bonds Supported by 9,10-Anthraquinone Carboxylate Ligands. Molecular and Electronic Structures and Ground State and Photoexcited State Redox Properties

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Table 1. Data Collection Parameters for **II**.

Compound	**II**
Chemical Formula	$C_{60}H_{52}Mo_2N_6O_{10}$
Formula Weight	1208.96
Temperature (K)	150(2)
Space Group	Triclinic, P-1
a (Å)	9.8000(2)
b (Å)	12.6442(2)
c (Å)	23.2653(3)
α (^{o})	100.197(1)
β (^{o})	100.351(1)
γ (^{o})	100.798(1)
V (Å^3)	2718.72(8)
Z	2
D_{calcd} (Mg/m^3)	1.477
Crystal Size (mm)	0.12 X 0.15 X 0.38
Theta range for data collection	1.68 to 27.47^o
μ,(Mo, Kα) (mm^{-1})	0.527
F(000)	1236
Reflections collected	75386
Unique reflections	12452 [R(int)= 0.052]
Completeness to theta max	99.9%
Data/restraints/parameters	12452 / 0 / 703
R1[a] (%) (all data)	4.49 (8.43)
wR2[b](%)(all data)	10.06 (11.08)
Goodness-of-fit on F^2	1.022
Largest diff. peak and hole (e Å^{-3})	1.253 and -0.402

[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

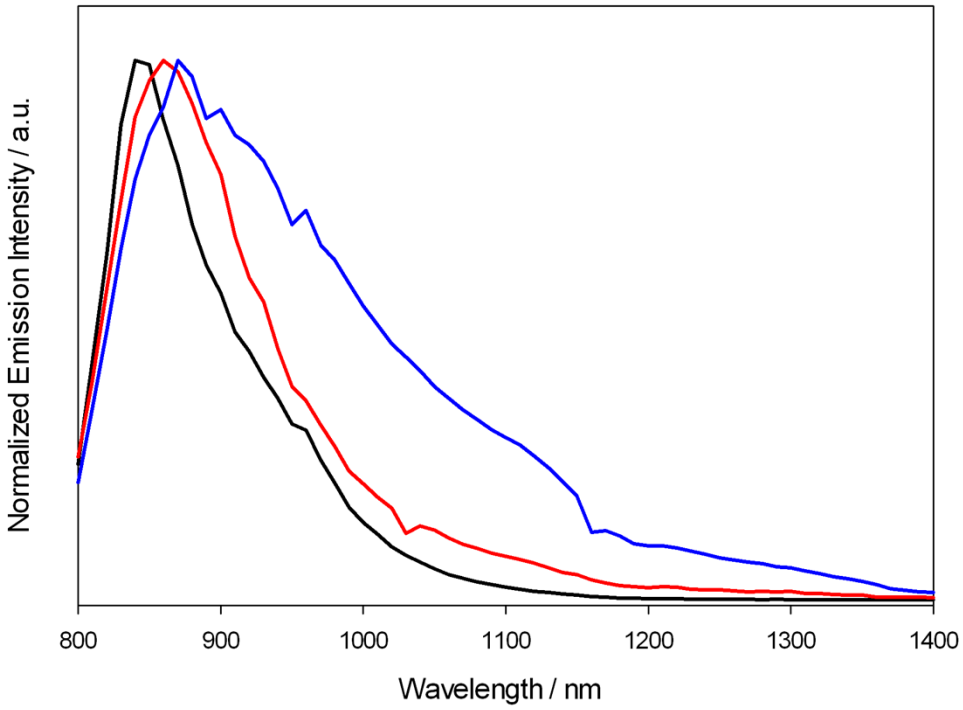

Figure S1. Emission spectra of $Mo_2(DAniF_3)(O_2C\text{-}2\text{-}ThCC)$ (black, λ_{exc} = 405 nm) and compound **II** (red, λ_{exc} = 405 nm), (blue, λ_{exc} = 658) in 2-MTHF at 77 K.

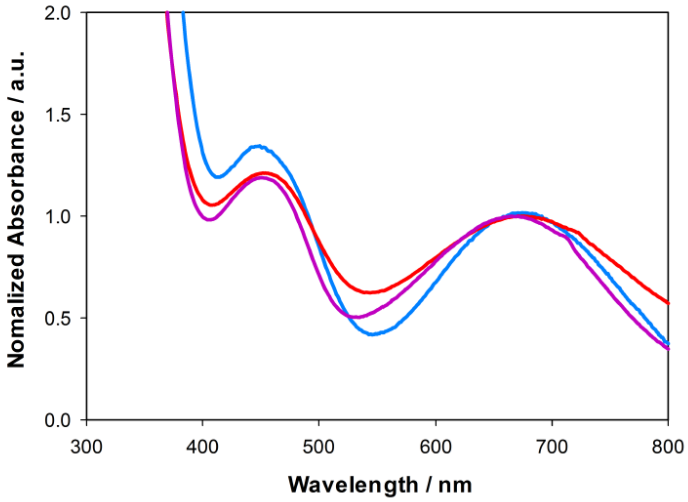

Figure S2. Absorption spectra of compound **II** in benzene (purple), CH_2Cl_2 (red) and THF (blue) at room temperature.

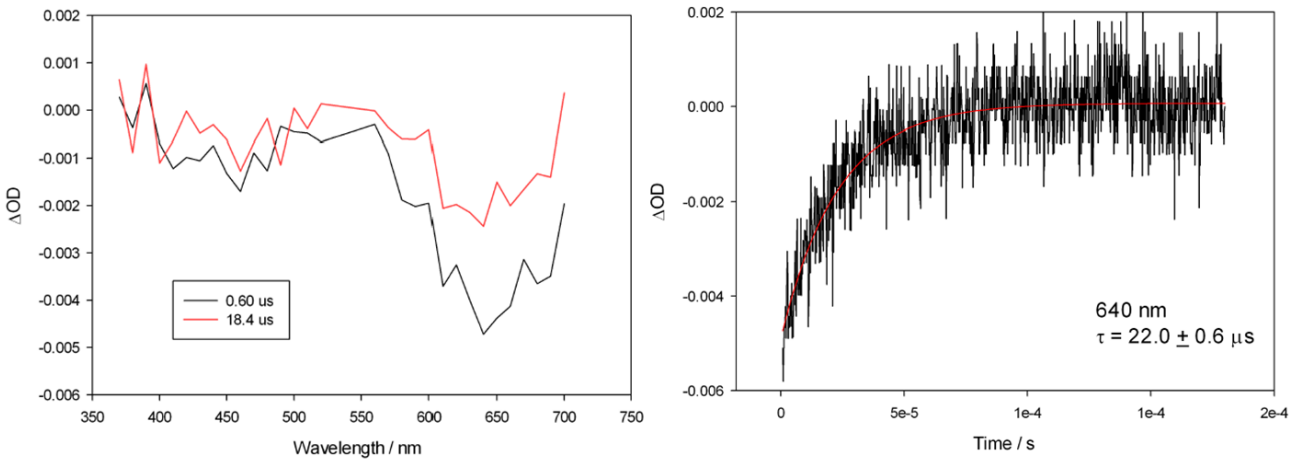

Figure S3. ns TA spectra and associated kinetic trace of compound **I** in THF, λ_{exc} = 532 nm.

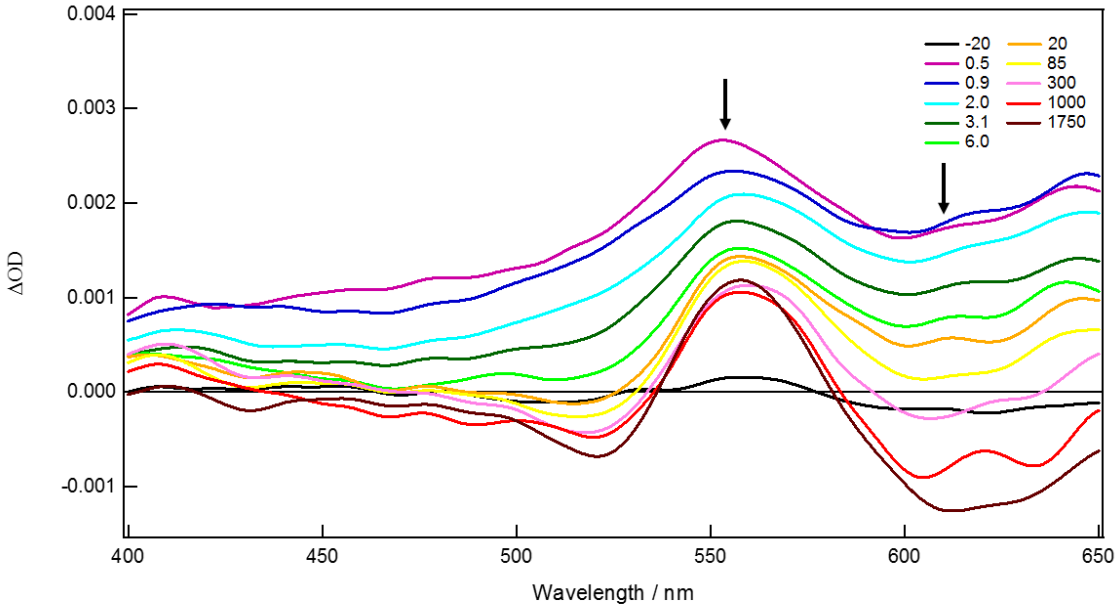

Figure S4. fs TA spectra of **II** in THF, λ_{exc} = 350 nm

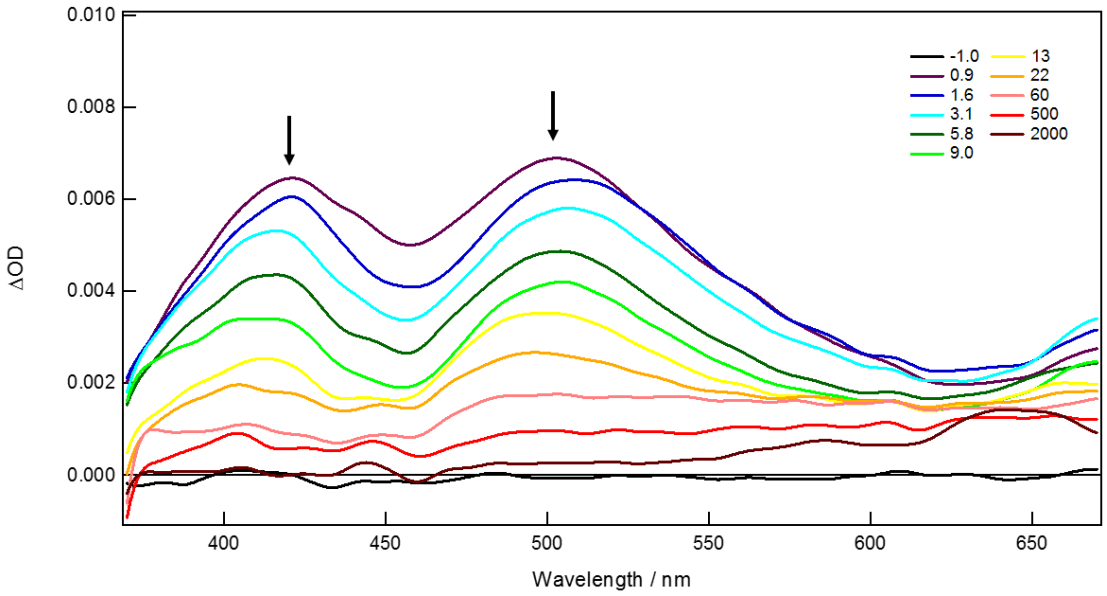

Figure S5. fs TA spectra of **II** in benzene, λ_{exc} = 350 nm

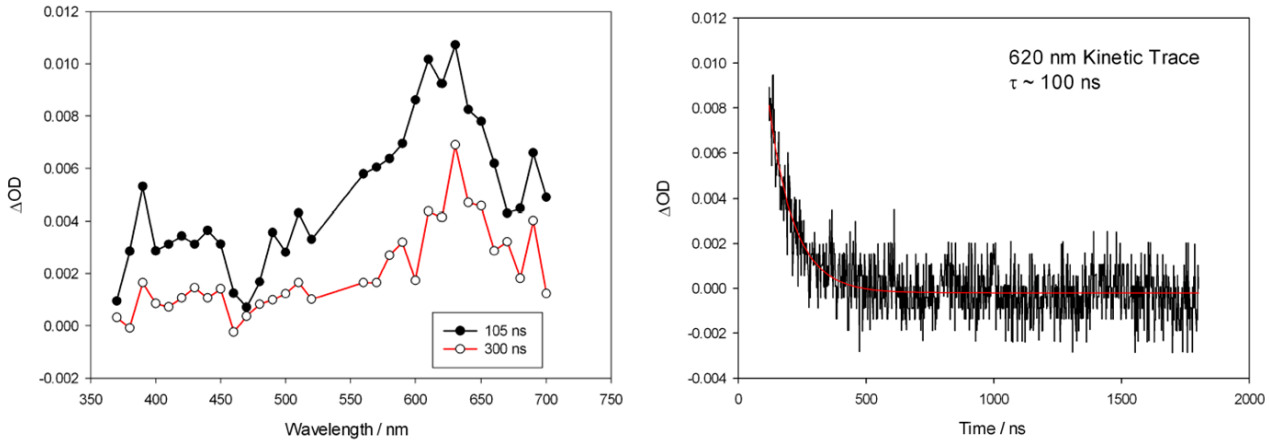

Figure S6. ns TA spectra and associated kinetic trace of compound **II** in benzene, λ_{exc} = 355 nm

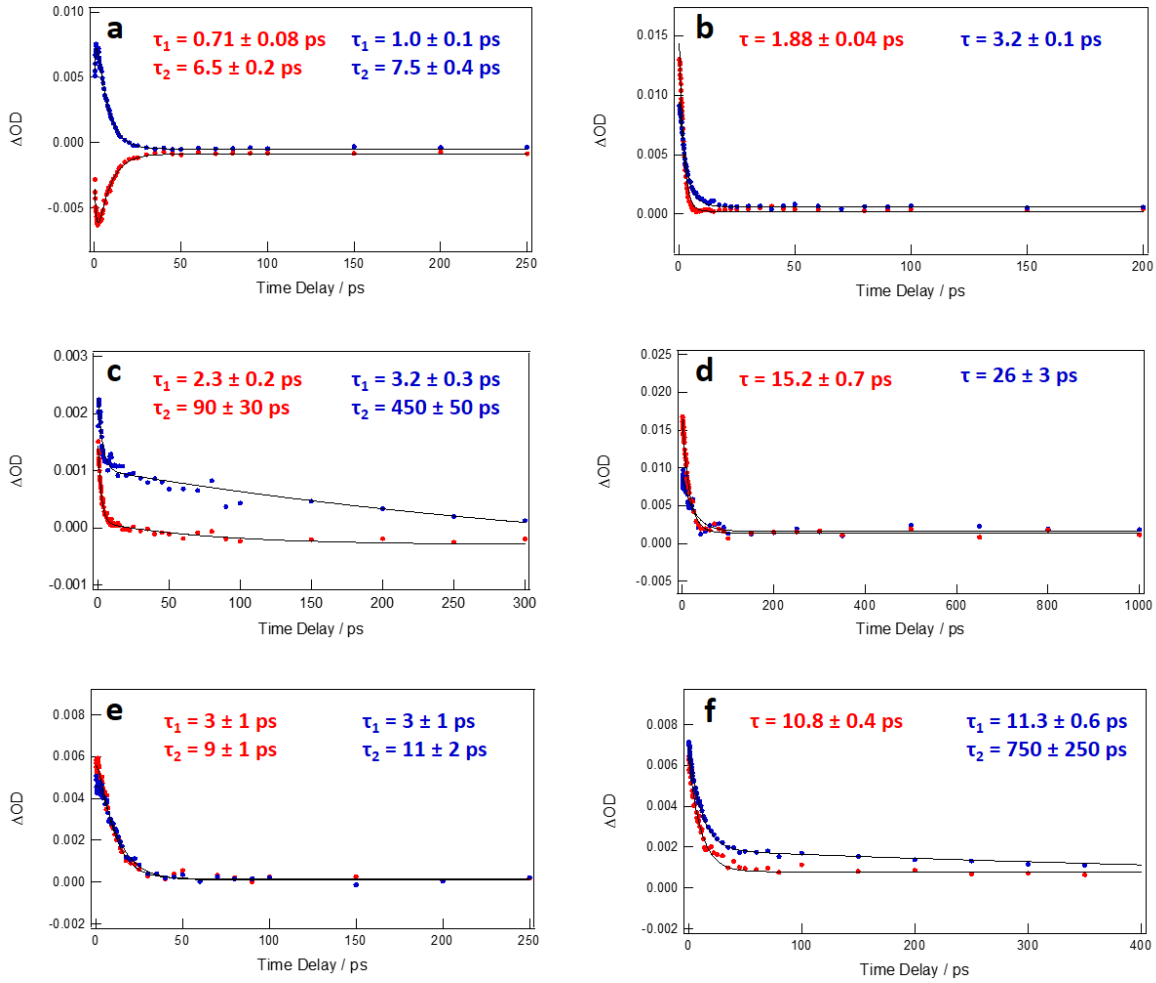

Figure S7. Kinetic traces for fs TA measurements: (a) Compound **I** in THF, λ_{exc} 675 nm, (b) Compound **II** in THF, λ_{exc} = 675 nm, (c) Compound **II** in THF, λ_{exc} = 350, (d) Compound **II** in toluene, λ_{exc} = 675, (e) and (f) Compound **II** in benzene, λ_{exc} = 675 and 350 nm respectively.

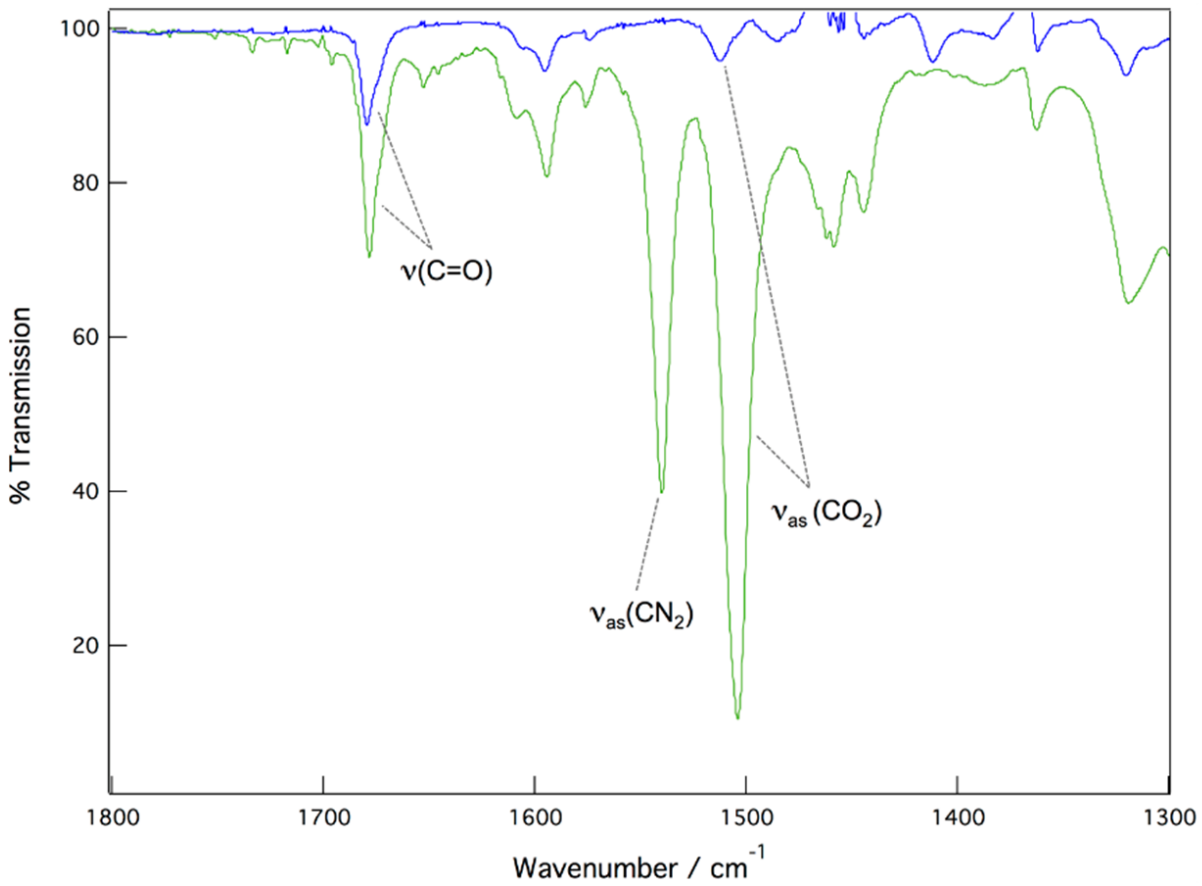

Figure S8. Ground-state infrared spectra of compound **I** (blue) and **II** (green) in THF at room temperature.

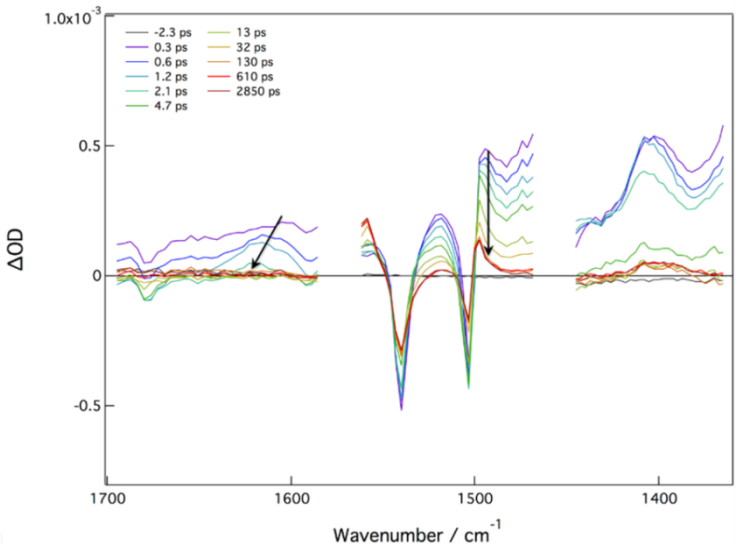

Figure S9. fs TRIR spectra of compound **II** in THF, λ_{exc} = 400 nm.

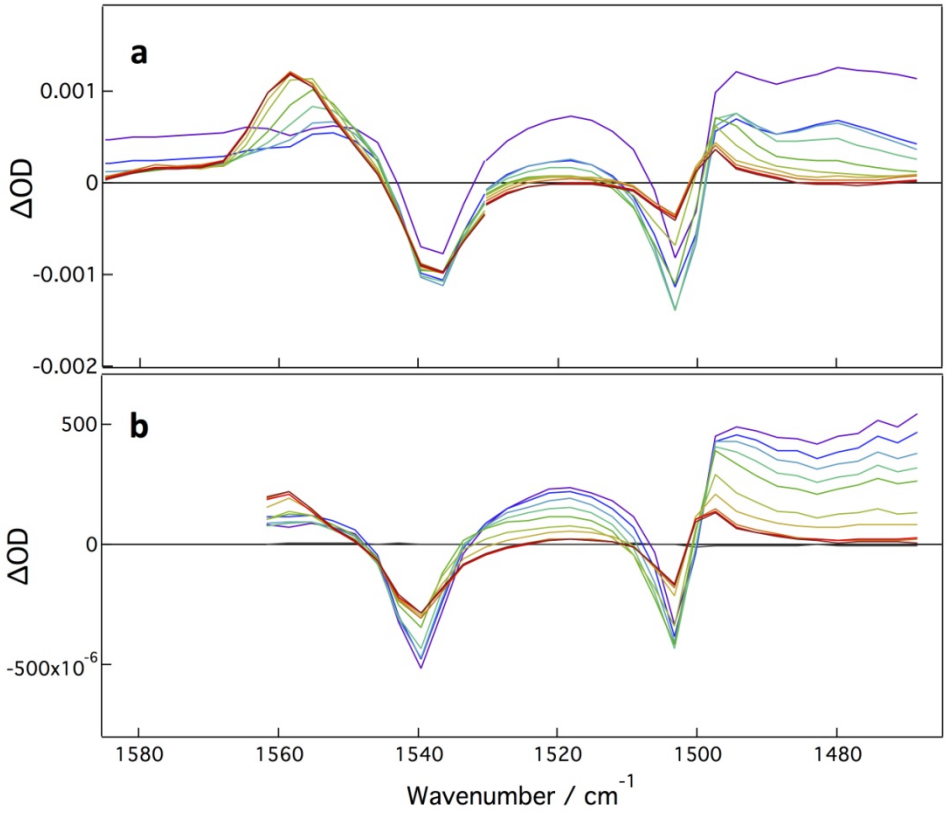

Figure S10. Comparison of long-lived features (orange trace) in TRIR spectra of $Mo_2(DAniF)_3(O_2C\text{-}C{\equiv}C\text{-}C_6H_4)$ (a) and compound **II** (b).

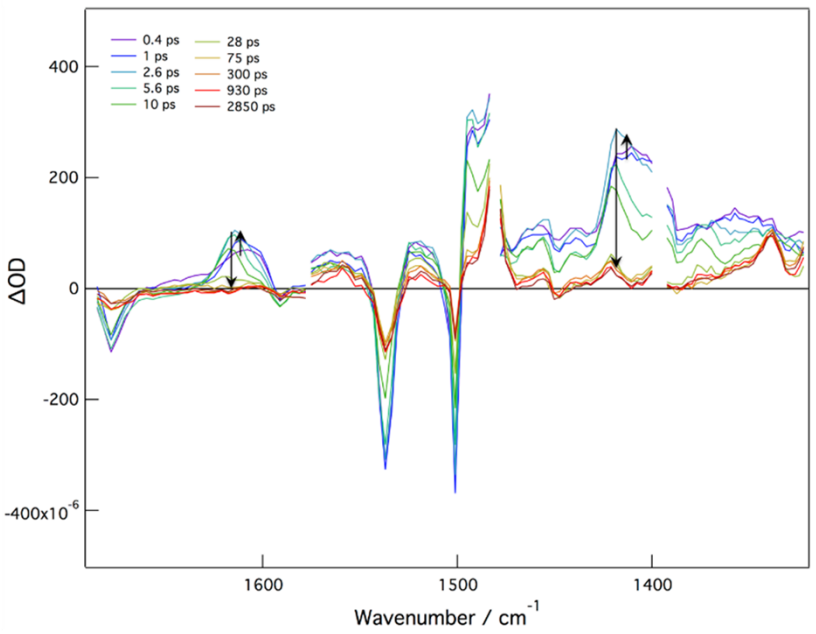

Figure S11. fs TRIR spectra of compound **II** in benzene, λ_{exc} = 400 nm.

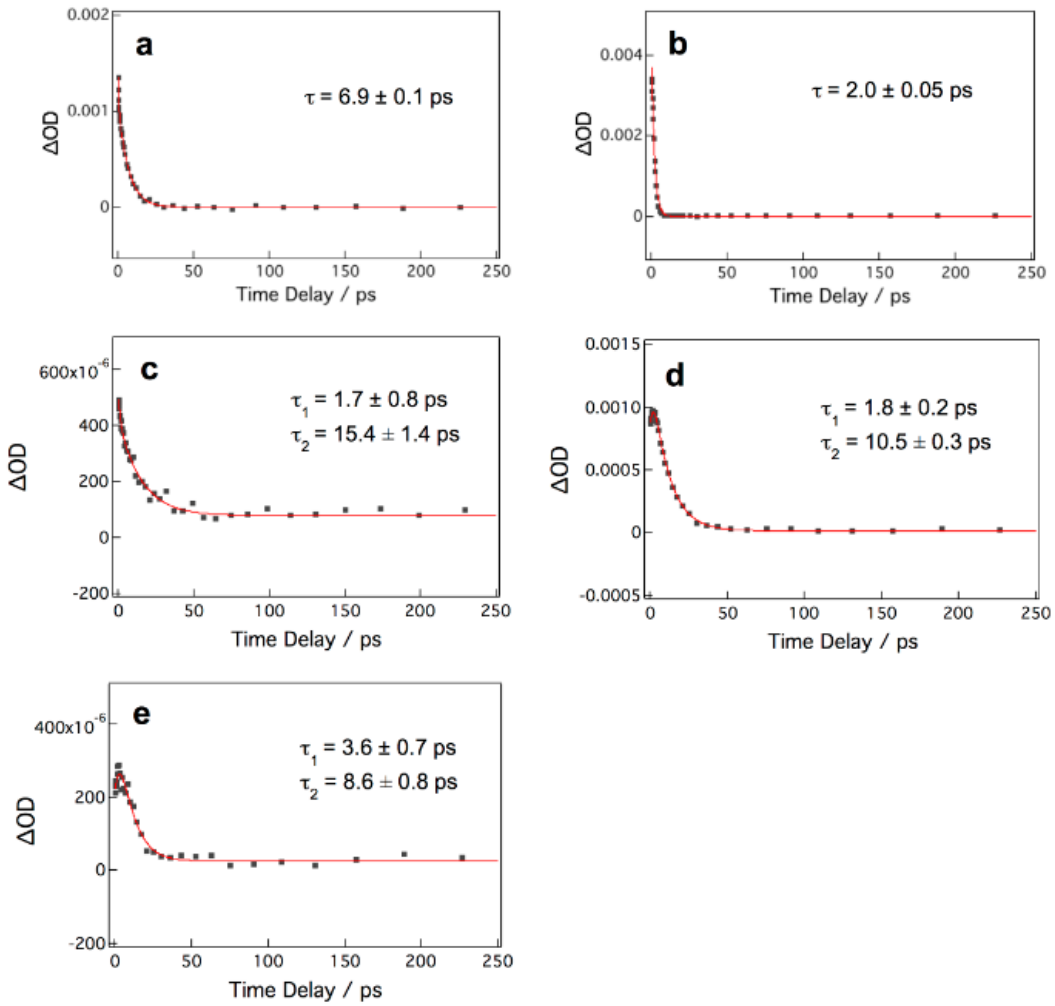

Figure S12. Kinetic traces for fs TRIR measurements: (a) Compound **I** in THF, λ_{exc} 675 nm, (b) and (c) Compound **II** in THF, λ_{exc} = 675 and 400 nm respectively, (d) and (e) Compound **II** in benzene, λ_{exc} = 675 and 400 nm respectively.