Electronic Supplementary Material (ESI) for Dalton Transactions
This journal is © The Royal Society of Chemistry 2012

Supporting Information

Manuscript: Photophysical Properties of MM Quadruply Bonded Complexes (M = Mo, W) Supported by Carboxylate Ligands: Charge Delocalization and Dynamics in S_1 and T_1 States

Authors: Brian G. Alberding, Samantha E. Brown-Xu, Malcolm H. Chisholm*, Terry L. Gustafson, Carly R. Reed, Vesal Naseri

Compound	**1**
Chemical Formula	$C_{84}H_{92}Mo_2O_{10}S_2$
Formula Weight	1517.58
Temperature (K)	180(2)
Space Group	Monoclinic, $P2_1/n$
a (Å)	9.7536(1)
b (Å)	14.6021(1)
c (Å)	26.2150(2)
α (^{o})	
B (^{o})	94.0908(2)
γ (^{o})	
V (Å^3)	3724.11(5)
Z	2
D_{calcd} (Mg/m^3)	1.353
Crystal Size (mm)	0.35 X 0.15 X 0.12
Theta range for data collection	2.59 to 26.37^o
μ,(Mo, Kα) (mm^{-1})	0.452
Reflections collected	14852
Unique reflections	7605 [R(int)= 0.0192]
Completeness to theta	(26.37) 99.9%
Data/restraints/parameters	7605 / 0 / 451
R1[a] (%) (all data)	3.05 (4.25)
wR2[b](%)(all data)	7.04 (7.51)
Goodness-of-fit on F^2	1.024
Largest diff. peak and hole (e Å^{-3})	0.707 and -0.578

[a] $R1 = \Sigma \; | |F_o|-|F_c| | \; / \; \Sigma \; |F_o|$

[b] $wR2 = \{ \Sigma \; [w(F_o^2-F_c^2)^2] \; / \; \Sigma \; [w(F_o^2)^2] \; \}^{1/2}$

Table S1. Select crystallographic information from structure **1**.

This journal is © The Royal Society of Chemistry 2012

Compound **1**			
Mo(1)-O(4)	2.1022(15)	Mo(1)-O(3)	2.5007(18)
Mo(1)-O(1)#1	2.1160(14)	O(1)-C(1)	1.270(2)
Mo(1)-Mo(1)#1	2.1164(6)	O(1)-Mo(1)#1	2.1160(14)
Mo(1)-O(2)	2.1184(14)	O(2)-C(1)	1.273(2)
Mo(1)-O(3)#1	2.1243(15)	O(3)-C(18)	1.272(2)
O(3)-Mo(1)#1	2.1243(15)	C(2)-C(3)	1.193(3)
O(4)-Mo(1)-O(1)#1	90.68(5)	O(1)#1-Mo(1)-O(2)	176.69(5)
O(4)-Mo(1)-Mo(1)#1	91.44(4)	Mo(1)#1-Mo(1)-O(2)	90.41(4)
O(1)#1-Mo(1)-Mo(1)#1	92.88(4)	O(4)-Mo(1)-O(3)	90.36(7)
O(4)-Mo(1)-O(2)	88.84(5)	C(2)-C(3)-C(4)	174.7(2)
C(18)-O(4)-Mo(1)	118.15(12)	O(1)-C(1)-O(2)	123.31(18)

Table S2. Select bond lengths (Å) and bond angles (°) for compounds **1**

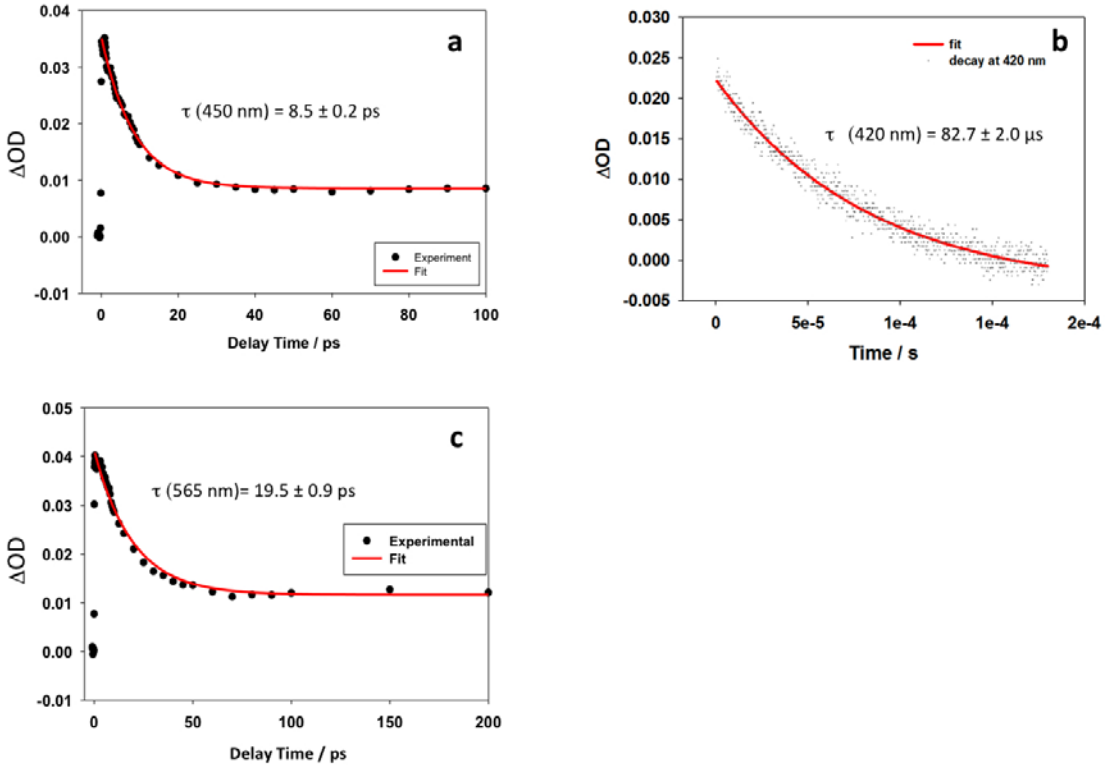

Fig. S1 (a) Kinetic trace from fs TA of **1** monitored at 450 nm, λ_{ex} = 514 nm; (b) Kinetic trace from ns TA of **1** monitored at 420 nm, λ_{ex} = 532 nm; (c) Kinetic trace from fs TA of **2** monitored at 565 nm, λ_{ex} = 675 nm.

This journal is © The Royal Society of Chemistry 2012

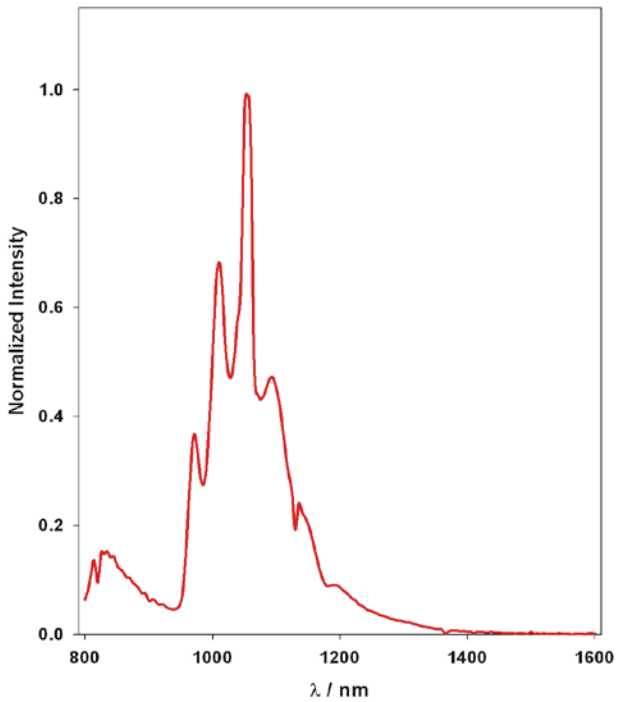

Fig. S2 Near-IR emission of **1** recorded in 2-methyl THF at 77 K.

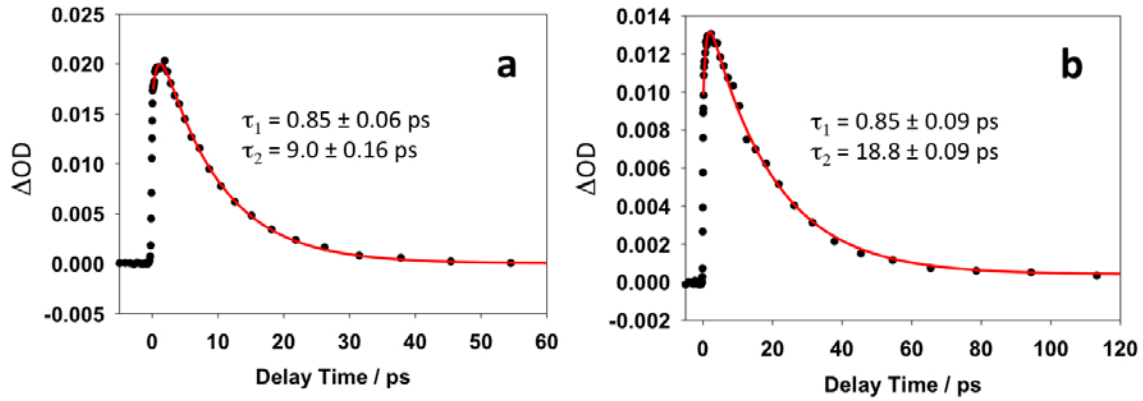

Fig. S3 (a) Kinetic trace from fs TRIR of **1** monitored at 2110 cm^{-1}, λ_{ex} = 514 nm; (b) Kinetic trace from fs TRIR of **2** monitored at 2150 cm^{-1}, λ_{ex} = 675 nm.