

Electronic Supplementary Information

Record luminescence characteristics of $[\text{Mo}_6\text{X}_8(\text{n-C}_3\text{F}_7\text{COO})_6]^{2-}$ (X = Br, I)

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Table S1. Selected bond distances (Å) and valence angles (°) of 1a, 2, and 3

Complex	1	2	3
M-M	2.59516(16)-2.60230(16)	2.6222(5)-2.6289(5)	2.6584(4)-2.6658(4)
M- μ_3 -X	2.4637(3)- 2.4878(3)	2.5885(5)-2.6179(5)	2.7583(3)-2.7880(3)
M-O	2.0952(10)-2.1082(10)	2.104(3)- 2.119(3)	2.120(2)-2.141(2)
C-O(M)	1.2775(17)-1.2852(17)	1.277(5)-1.288(5)	1.261(4)-1.269(4)
C=O	1.2094(18)-1.2123(17)	1.205(5)-1.215(5)	1.220(4)-1.215(4)
M-O-C	126.28(9)-134.56(9)	128.0(3)-135.5(3)	129.6(2)-137.1(2)
O-C-O	129.36(14)-130.18(14)	129.7(4)-130.6(4)	130.2(3)-131.4(3)

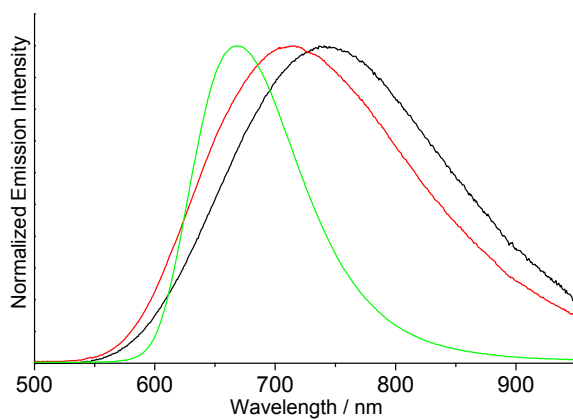


Fig S1. Emission spectra for **1** (black), **2** (red), and **3** (green) in the solid state at 298 K.

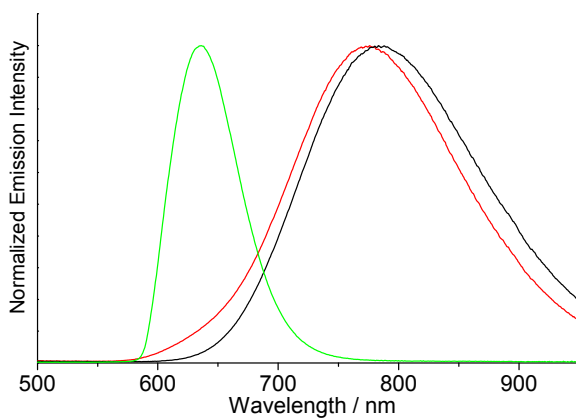
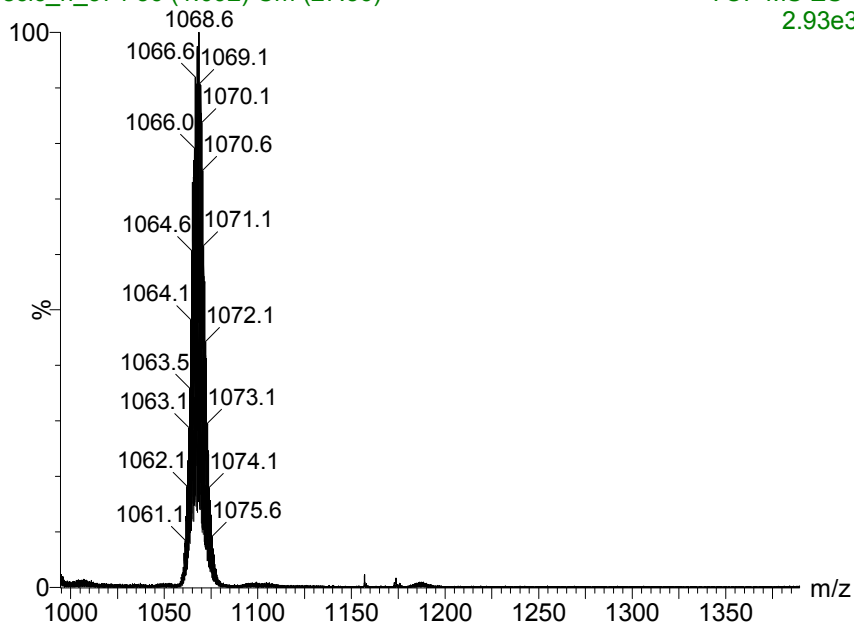


Fig. S2. Emission spectra for **1** (black), **2** (red), and **3** (green) in the solid state at 80 K.

XP171 (PPh₄)₂Mo₆Cl₈(O₂CC₃F₇)₆ scan neg MeCN conos crecie

scic_rl_374 56 (1.092) Cm (27:56)

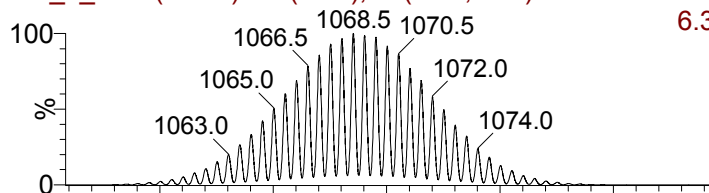
TOF MS ES-
2.93e3



XP171 (PPh₄)₂Mo₆Cl₈(O₂CC₃F₇)₆ scan neg MeCN cc

scic_rl_374 (0.019) Cu (0.20); Is (1.00,0.01) Mo₆Cl₈O₁₂C₂₄F₄₂

6.35e11



scic_rl_374 39 (0.768) Sm (Mn, 2x2.00); Cm (28:43)

1.25e3

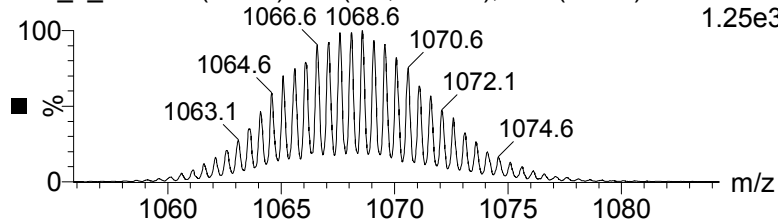


Fig. S3. ESI-MS of **1** at the negative voltage. Top: the spectrum in CH₃CN. Bottom: calculated and observed isotopic patten for the peak attributable to [Mo₆Cl₈(C₃F₇COO)₆]²⁻.