Supplementary Material (ESI) for Dalton Transactions

Host-Guest adaptability within oxothiomolybdenum wheels: Structures, studies in solution and DFT calculations

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Supporting Information

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Table S1: Selected bond lengths in $(NMe_4)_2[Mo_{12}\text{-Adip}]$, $K_2[Mo_{12}\text{-Sub}]$ and $(NMe_4)_2[Mo_{14}\text{-Azel}]$.

$(NMe_4)_2[Mo_{12}\text{-Adip}]$		$K_2[Mo_{12}\text{-Sub}]$		$(NMe_4)_2[Mo_{14}\text{-Azel}]$	
Mo(1)-O(1)	1.693(5)	Mo(1)-O(1)	1.683(2)	Mo(1)-O(1)	1.677(3)
Mo(1)-O(13)	2.103(3)	Mo(1)-O(4)	2.0624(11)	Mo(1)-O(8)	2.106(3)
Mo(1)-S(1)	2.3209(11)	Mo(1)-S(1)	2.2922(5)	Mo(1)-S(2)	2.3083(12)
Mo(1)-O(19)	2.336(4)	Mo(1)-Mo(2)	2.8148(3)	Mo(1)-S(1)	2.3212(11)
Mo(1)-Mo(2)	2.7936(7)	Mo(2)-O(2)	1.675(2)	Mo(1)-O(15)	2.566(3)
Mo(2)-O(2)	1.703(5)	Mo(2)-O(5)	2.0807(14)	Mo(1)-Mo(2)	2.8284(5)
Mo(2)-O(14)	2.102(3)	Mo(2)-S(1)	2.3225(5)	Mo(2)-O(2)	1.679(3)
Mo(2)-S(1)	2.3269(12)	Mo(2)-Mo(3)	3.315(1)	Mo(2)-O(10)	2.062(3)
Mo(2)-O(20)	2.335(4)	Mo(3)-O(3)	1.686(2)	Mo(2)-O(9)	2.092(3)
Mo(3)-O(3)	1.693(5)	Mo(3)-O(5)	2.1052(14)	Mo(2)-S(2)	2.3130(11)
Mo(3)-O(14)	2.079(3)	Mo(3)-S(2)	2.3227(6)	Mo(2)-S(1)	2.3271(11)
Mo(3)-S(2)	2.3257(12)	Mo(3)-O(6)	2.328(3)	Mo(2)-O(16)	2.461(3)
Mo(3)-O(20)	2.416(4)	Mo(3)-Mo(3)	2.7993(5)	Mo(3)-O(3)	1.681(3)
Mo(3)-Mo(4)	2.8116(7)			Mo(3)-O(10)	2.066(3)
Mo(4)-O(4)	1.699(4)			Mo(3)-O(9)	2.077(3)
Mo(4)-O(15)	2.063(3)			Mo(3)-S(4)	2.3270(11)
Mo(4)-S(2)	2.3043(12)			Mo(3)-S(3)	2.3343(11)
Mo(5)-O(5)	1.675(4)			Mo(3)-O(17)	2.413(3)
Mo(5)-O(15)	2.069(3)			Mo(3)-Mo(4)	2.8240(5)
Mo(5)-S(3)	2.3071(11)			Mo(4)-O(4)	1.686(3)
Mo(5)-Mo(6)	2.8055(7)			Mo(4)-O(11)	2.100(3)
Mo(6)-O(6)	1.710(4)			Mo(4)-O(12)	2.130(3)

Mo(6)-O(16) 2.046(3)	Mo(4)-O(18) 2.302(3)
Mo(6)-S(3) 2.3111(11)	Mo(4)-S(4) 2.3200(11)
Mo(7)-O(7) 1.693(4)	Mo(4)-S(3) 2.3243(11)
Mo(7)-O(16) 2.098(3)	Mo(5)-O(5) 1.670(3)
Mo(7)-O(21) 2.304(4)	Mo(5)-O(11) 2.093(3)
Mo(7)-S(4) 2.3243(11)	Mo(5)-O(12) 2.118(3)
Mo(7)-Mo(8) 2.8027(7)	Mo(5)-S(5) 2.3095(11)
Mo(8)-O(8) 1.700(5)	Mo(5)-S(6) 2.3234(10)
Mo(8)-O(17) 2.115(3)	Mo(5)-O(18) 2.465(3)
Mo(8)-O(22) 2.272(4)	Mo(5)-Mo(6) 2.8164(5)
Mo(8)-S(4) 2.3282(11)	Mo(6)-O(6) 1.679(3)
Mo(9)-O(9) 1.672(5)	Mo(6)-O(13) 2.057(3)
Mo(9)-O(17) 2.078(3)	Mo(6)-O(14) 2.062(3)
Mo(9)-S(5) 2.3285(12)	Mo(6)-S(6) 2.3030(12)
Mo(9)-Mo(10) 2.8259(7)	Mo(6)-S(5) 2.3054(11)
Mo(10)-O(10) 1.681(5)	Mo(7)-O(7) 1.664(4)
Mo(10)-O(18) 2.122(3)	Mo(7)-O(14) 2.050(3)
Mo(10)-S(5) 2.3289(13)	Mo(7)-O(13) 2.064(3)
Mo(10)-O(23) 2.471(5)	Mo(7)-S(7) 2.3006(12)
Mo(11)-O(11) 1.699(4)	Mo(7)-Mo(7)#1 2.8069(7)
Mo(11)-O(18) 2.092(3)	
Mo(11)-S(6) 2.3191(12)	
Mo(11)-O(23) 2.542(5)	
Mo(12)-O(12) 1.675(5)	
Mo(12)-O(13) 2.059(3)	

Mo(12)-S(6)	2.3127(11)

Figure S1: 300 Mhz ^{1}H NMR spectra of $[Mo_{12}\text{-Adip}]^{2-}$ (b), $[Mo_{12}\text{-Sub}]^{2-}$ (d) and $[Mo_{14}\text{-Azel}]^{2-}$ (f) compared to those of free $Adip^{2-}$(a), Sub^{2-} (c) and $Azel^{2-}$ (e) in D_2O.

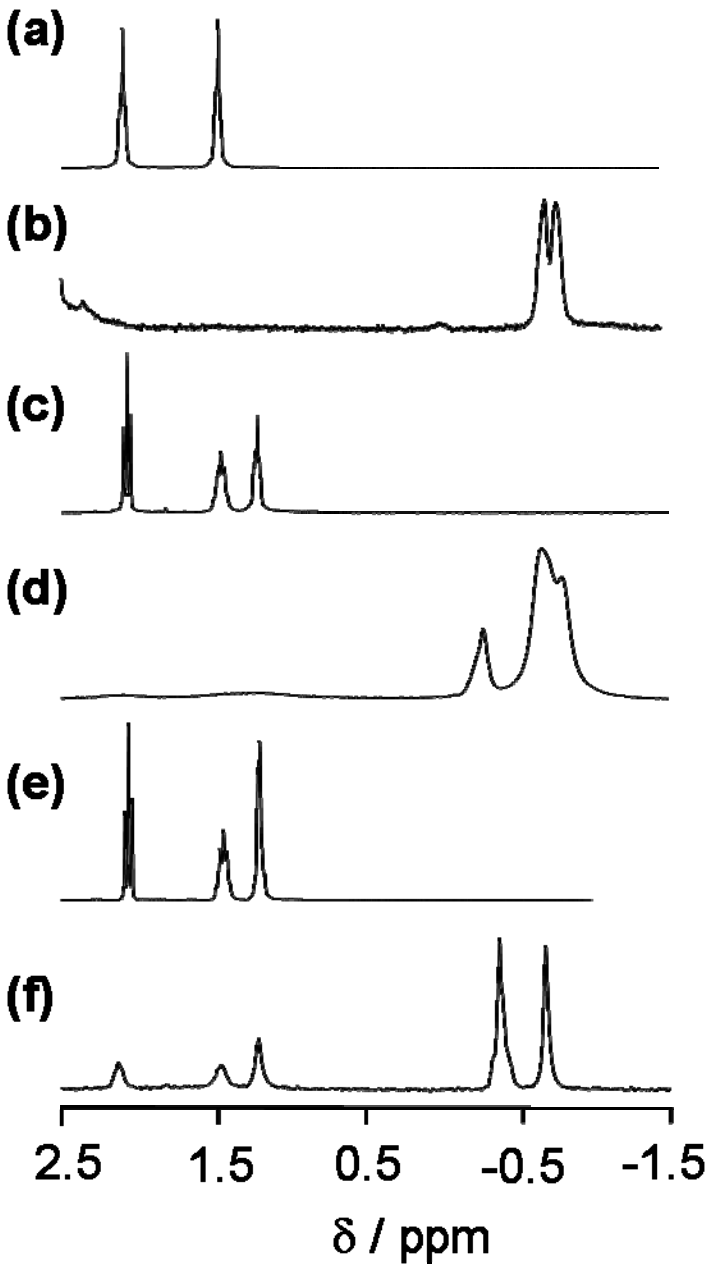

Figure S2: 300 Mhz ^{1}H NMR spectra of $[Mo_{12}\text{-Adip}]^{2-}$ and $[Mo_{12}\text{-Sub}]^{2-}$ in [D6]DMSO

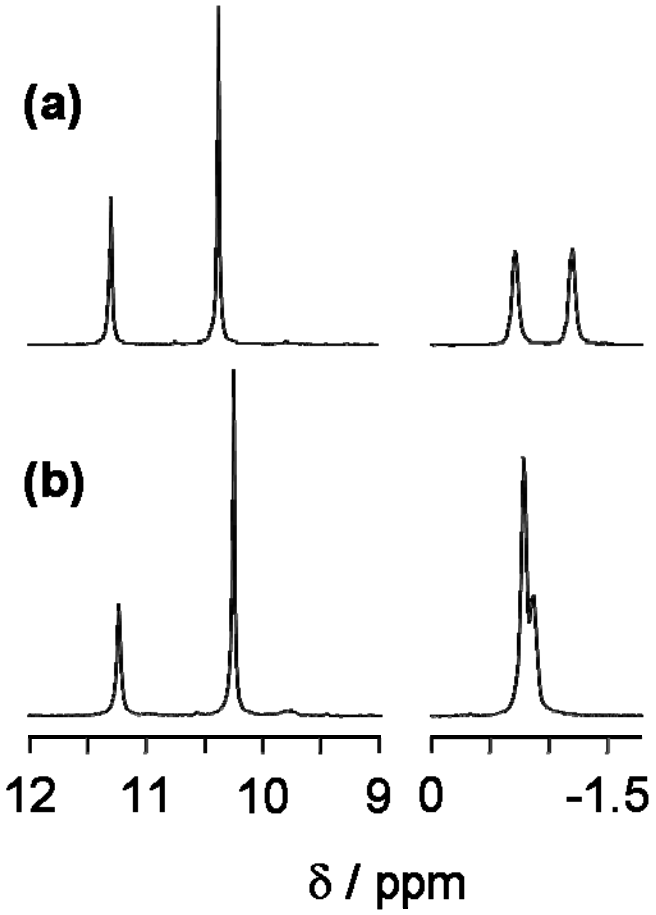

Figure S3: Evolution of proportions of free Sub^{2-} and Mo_{12}-Sub]$^{2-}$ as a function of temperature in D_2O. Inset:Van't Hoff plot as a function of temperature.