

SUPPORT INFORMATION

Table S1. Summary of data collection and structure refinement.

Identification	$[(\text{MoO}_2)_2(\text{BPA})_2(\mu\text{-O})]$
Formula	$\text{C}_{26}\text{H}_{26}\text{Mo}_2\text{N}_4\text{O}_7$
Fw (g mol ⁻¹)	698.39
T (K)	291(2)
λ (Å)	0.71073
Crystal system	Monoclinic
Space group	$P2_1/n$
a (Å)	11.7279(5)
b (Å)	15.2529(5)
c (Å)	14.7858(6)
α (°)	90
β (°)	90.9290(10)
γ (°)	90
Volume (Å ³)	2644.60(18)
Z	4
ρ_{calc} (Mg m ⁻³)	1.754
μ (mm ⁻¹)	1.001
F(000)	1400
θ range(°)	2.20-26.40
Index ranges	$-14 \leq h \leq 14$ $-19 \leq k \leq 19$ $-18 \leq l \leq 18$
Data collected	47048
Independent reflections	5404
R_{int}	0.0273
Refinement method	Full matrix least squares on F^2
Data / restraints / parameters	5404/2/360
GOF on F^2	1.200
R1, wR2 [$I > 2\sigma(I)$]	0.0289; 0.0681
R1, wR2 (all)	0.0339; 0.0729
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e·Å ⁻³)	0.729; -0.821

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Internal standart: anthracene solution at concentration $2,5 \cdot 10^{-3}$ mol L⁻¹ in acetonitrile.

Standard solutions: Substrates (dibenzothiophene, diphenylsulfide and thioanisole) at concentrations showed at Table S2 in acetonitrile.

The injections at GC-MS were performed with mixture of 50 μ L of each standart solution of DBT, DPS and THIO and 450 μ L of internal standard solution.

Table S2. Substrate concentrations of standart solutions from analytical curves for sulfide quantification.

	Substrate concentration (mol. L ⁻¹)	Substrate (%)
1	$7.00 \cdot 10^{-2}$	100
2	$5.25 \cdot 10^{-2}$	75
3	$3.50 \cdot 10^{-2}$	50
4	$1.75 \cdot 10^{-2}$	25
5	$7.00 \cdot 10^{-4}$	1
6	$7.00 \cdot 10^{-5}$	0,1

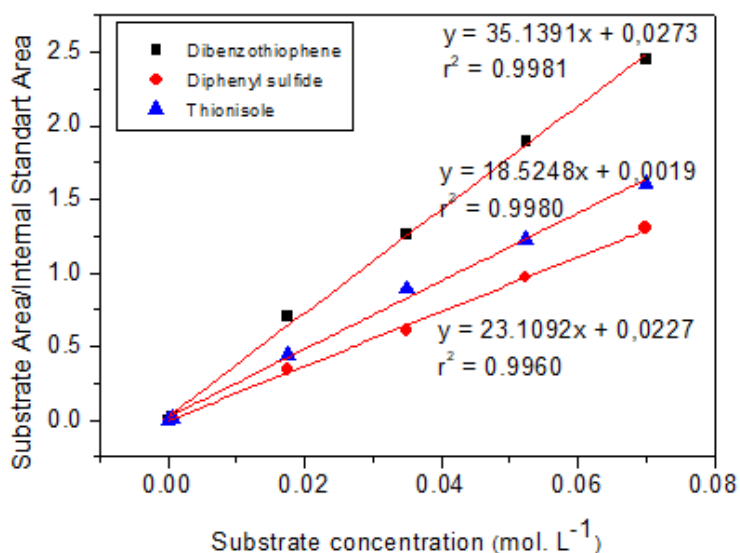


Figure S1. Calibration curves for quantification of sulfide conversion.

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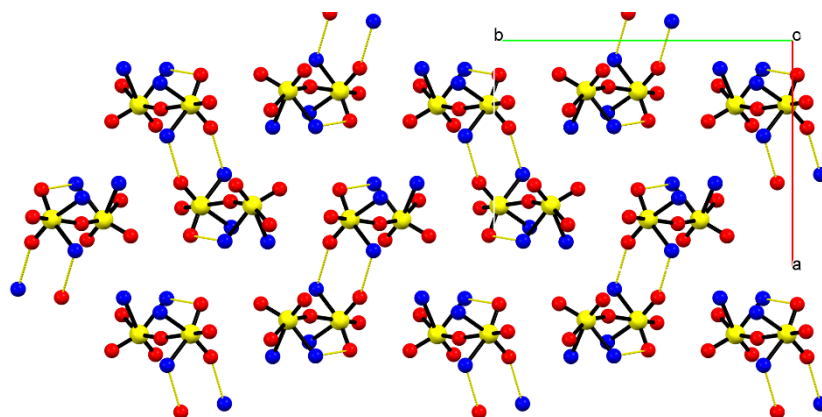


Figure S2. View of crystal packing along a direction evidencing intramolecular and intermolecular hydrogen bonds (yellow dashed line). Carbon and hydrogen atoms were omitted for clarity.

Table S3. Continuous shape measure values for $[(\text{MoO}_2)_2(\text{BPA})_2(\mu\text{-O})]$.

	Hexagon	Pentagonal pyramid	Octahedron	Trigonal prism	Johnson pentagonal pyramid J2
Mo1	31.815	29.013	0.903	16.010	32.247
Mo2	31.792	27.246	1.019	15.051	30.624

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Table S4. Comparison between calculated and crystal data bonding lengths of [(MoO₂)₂(BPA)₂(μ-O)] complex.

Bond	Calculated (Å)	Experimental (Å)	Difference (%)
Mo1-O1	1.92104	1.883(2)	2.02
Mo1-O2	1.97792	1.988(2)	-0.51
Mo1-O3	1.76865	1.720(2)	2.83
Mo1-O4	1.75754	1.700(2)	3.38
Mo1-N1	2.37838	2.335(2)	1.86
Mo1-N2	2.35036	2.356(2)	-0.24
Mo2-O1	1.93916	1.913(2)	1.37
Mo2-O5	1.98649	1.981(2)	0.28
Mo2-O6	1.75725	1.706(2)	3.00
Mo2-O7	1.75868	1.703(2)	3.27
Mo2-N3	2.35717	2.340(2)	0.73
Mo2-N4	2.36714	2.363(2)	0.18
O4-Mo1-O3	107.519	106.5(1)	0.96
O4-Mo1-O1	97.6476	99.94(9)	-2.29
O3-Mo1-O1	96.66481	98.18(8)	-1.54
O4-Mo1-O2	96.1737	95.33(9)	0.89
O3-Mo1-O2	98.88854	96.38(8)	2.60
O1-Mo1-O2	155.00681	154.92(8)	0.06
O4-Mo1-N1	89.91592	92.30(9)	-2.58
O3-Mo1-N1	162.42655	161.20(9)	0.76
O1-Mo1-N1	78.37178	78.59(8)	-0.28
O2-Mo1-N1	80.93174	81.05(7)	-0.15
O4-Mo1-N2	161.22231	162.79(9)	-0.96
O3-Mo1-N2	91.09937	90.01(9)	1.21
O1-Mo1-N2	82.18541	82.05(8)	0.17
O2-Mo1-N2	78.08493	77.63(7)	0.59
N1-Mo1-N2	71.59926	71.23(7)	0.52
Mo1-O1-Mo2	152.34313	157.8(1)	-3.46
O7-Mo2-O6	108.25566	107.4(1)	0.80
O7-Mo2-O1	95.99379	98.53(9)	-2.57
O6-Mo2-O1	100.14182	100.44(9)	-0.30
O7-Mo2-O5	93.12026	93.42(9)	-0.32
O6-Mo2-O5	96.48035	96.35(9)	0.14
O1-Mo2-O5	157.45752	155.38(8)	1.34
O7-Mo2-N3	94.2012	94.92(9)	-0.76
O6-Mo2-N3	157.01288	156.95(9)	0.04
O1-Mo2-N3	81.82891	81.39(8)	0.54
O5-Mo2-N3	76.96608	76.19(8)	1.02
O7-Mo2-N4	165.26334	164.59(9)	0.41
O6-Mo2-N4	86.3215	87.49(9)	-1.34
O1-Mo2-N4	83.16797	82.20(8)	1.18
O5-Mo2-N4	82.81413	80.68(8)	2.65
N3-Mo2-N4	71.09448	69.90(8)	1.71

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Table S5. Calculated atomic Mulliken charges for $[(\text{MoO}_2)_2(\text{BPA})_2(\mu\text{-O})]$ complex.

Atoms numbers correspond to the crystal structure data of Figure 2.

Atom	Mulliken Charges
Mo1	1.284
Mo2	1.242
O1	-0.766
O2	-0.563
O3	-0.567
O4	-0.500
O5	-0.548
O6	-0.522
O7	-0.486
N1	-0.469
N2	-0.273
N3	-0.520
N4	-0.273

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Table S6. FITR mainly wavenumber bands (cm^{-1}) in the vibration spectra of the HBPA ligand and $[(\text{MoO}_2)_2(\text{BPA})_2(\mu\text{-O})]$.

HBPA	Mo complex	Group vibration
-	3438	$\nu\text{O-H}$ (water)
3263	3236, 3176	$\nu\text{N-H}$ (primary amine)
3039	3073	$\nu\text{C-H}$ (aromatic)
2931	2913	$\nu\text{C-H}$ (aliphatic, symmetrical)
2859	-	$\nu\text{C-H}$ (aliphatic, unsymmetrical)
1593, 1456, 1429	1605, 1480, 1448	$\nu\text{C=C}$, $\nu\text{C=N}$ (double bonds in aromatics)
1356	-	$\delta\text{O-H}$ (phenol)
-	1024	$\nu\text{N-Mo}$
-	907	$\nu\text{Mo=O}$ (dioxomolybdenum)
-	743, 759	$\nu\text{Mo-O-Mo}$
	471	$\nu\text{N-Mo}$

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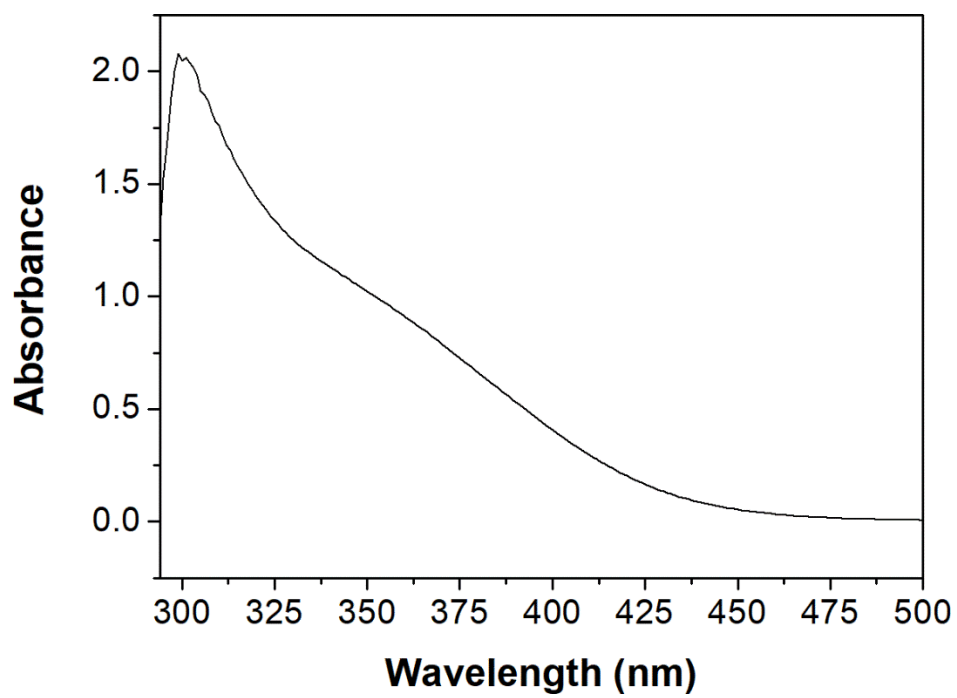


Figure S3. Electronic spectrum of Mo(VI) complex in DMSO solution of 2.86×10^{-4} mol/dm³.

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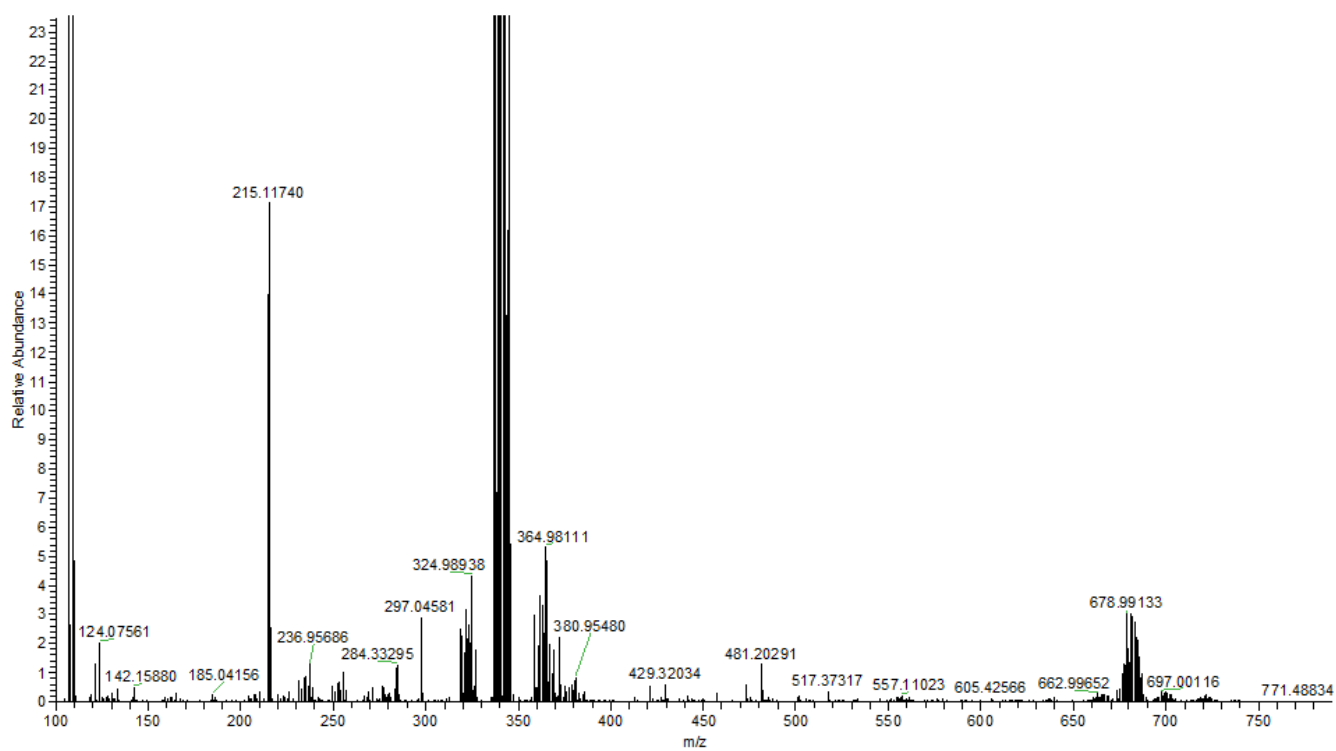


Figure S4. Experimental ESI-(+)-MS for $[(\text{MoO}_2)_2(\text{BPA})_2(\mu\text{-O})]^+$ in methanol solution.

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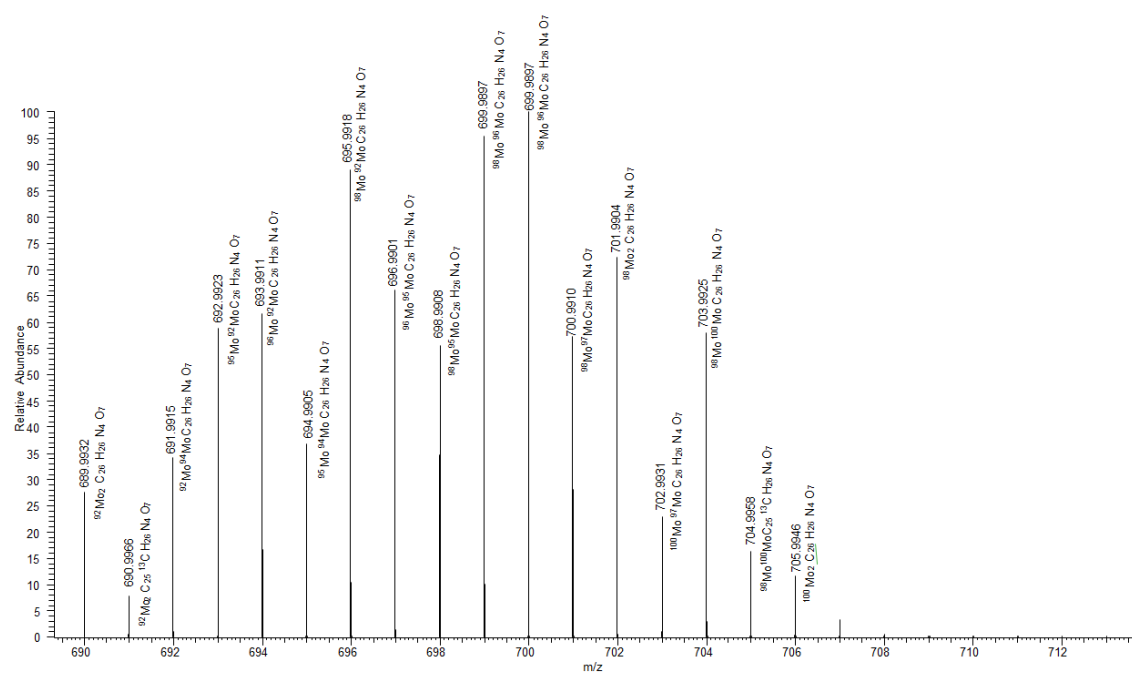
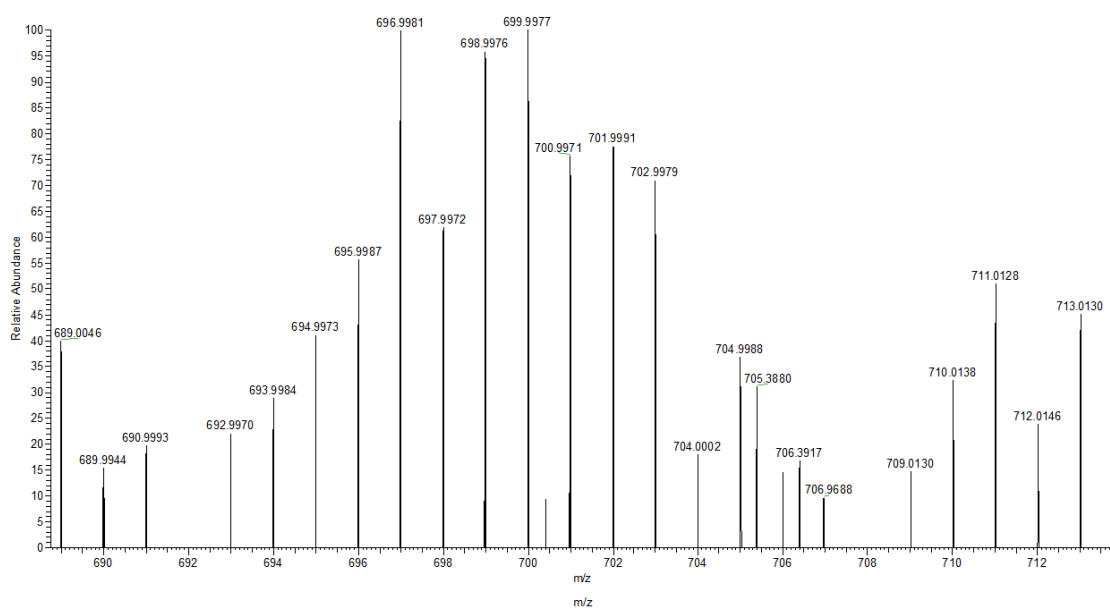


Figure S5. Experimental (top) and calculated (bottom) isotopic pattern for $[(\text{MoO}_2)_2(\text{BPA})_2(\mu\text{-O})]^+$.

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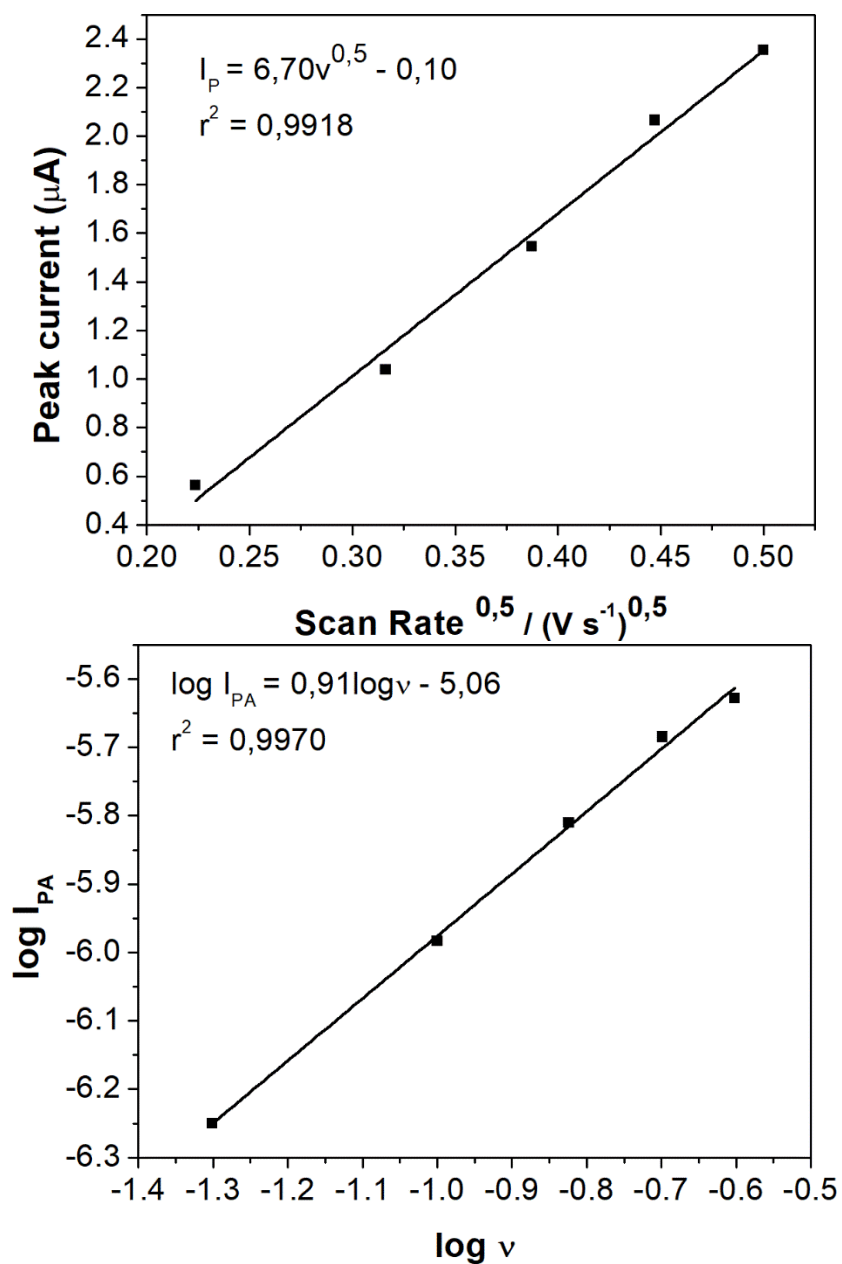


Figure S6. The linear dependence of I_{pa} vs. $v^{1/2}$ of anodic peak (E_{a1}) (top) and the linear relationship between the logarithm of I_{pa} and the logarithm of v (bottom).