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New polymeric, dimeric and mononuclear dioxidomolybdenum(VI) complexes with an ONO donor ligand: Crystal structures, DFT calculations, Catalytic performance and Protein binding study of the ligand

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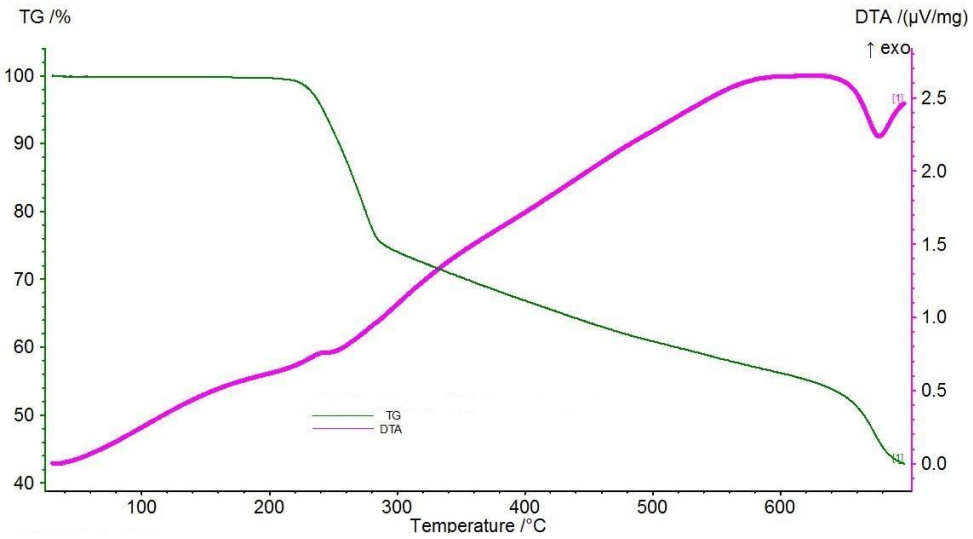

Fig. S1 TG-DT curve of complex **1** under N_2 atmosphere

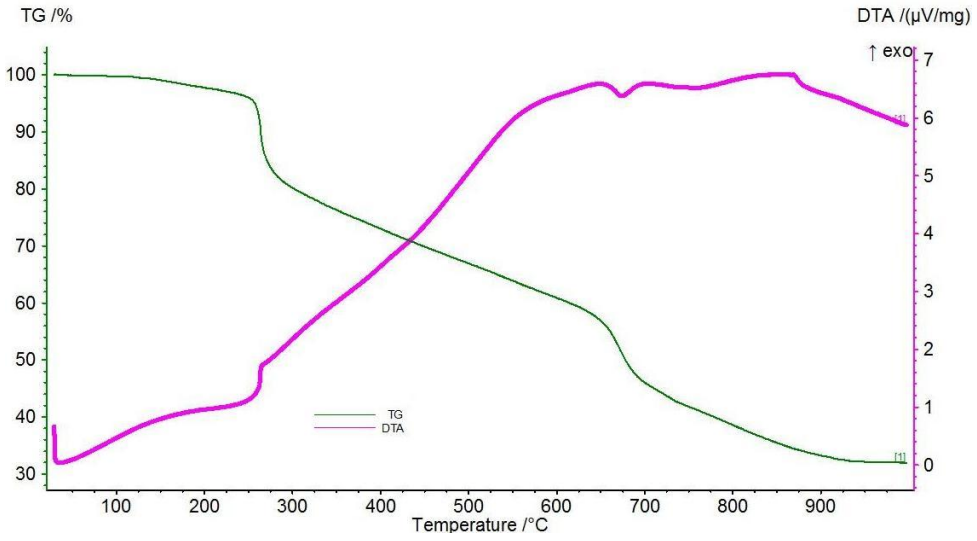

Fig. S2 TG-DT curve of complex **2** under N_2 atmosphere

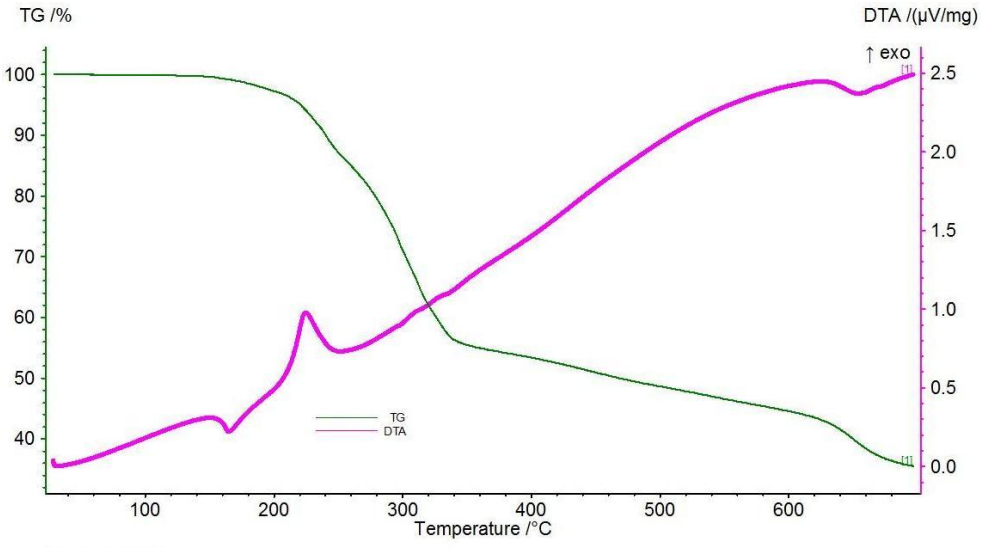

Fig. S3 TG-DT curve of complex **4** under N_2 atmosphere

Table S1

X-ray and calculated (DFT/B3LYP methodology) bond lengths of complexes **1**-**5**

Bond Distances (Å)	**1**		**2**		**3**		**4**			**5**	
	obs	calc	obs	calc	obs	calc	obs A	obs B[c]	calc	obs	calc
Mo(1)-O(3)	1.712(4)	1.748	1.693(5)	1.746	1.694(4)	1.739	1.700(2)	1.704(3)	1.740	1.691(2)	1.737
Mo(1)-O(4)	1.699(4)	1.740	1.708(5)	1.733	1.695(4)	1.745	1.706(2)	1.712(3)	1.750	1.713(2)	1.739
Mo(1)-O(2)	1.949(4)	1.965	1.934(5)	1.972	1.939(4)	1.986	1.943(2)	1.942(3)	.1.987	1.947(2)	1.999
Mo(1)-O(1)	1.957(4)	1.984	1.998(5)	1.999	1.982(4)	2.006	1.994(2)	1.983(2)	2.006	2.002(2)	2.004
Mo(1)-N(3)	2.201(5)	2.251	2.222(5)	2.239	2.229(5)	2.275	2.239(3)	2.226(3)	2.273	2.227(2)	2.285
Mo(1)-X[a]	2.482(4)	2.661	2.553(6)	2.972	2.451(5)	2.512	2.366(3)	2.366(3)	2.450	2.297(2)	2.403
C(7)-O(1)	1.344(7)	1.363	1.334(8)	1.360	1.332(7)	1.357	1.334(4)	1.338(4)	1.355	1.328(3)	1.351
C(7)-N(2)	1.294(8)	1.316	1.297(9)	1.314	1.293(7)	1.323	1.297(4)	1.294(5)	1.323	1.304(3)	1.328
N(2)-N(3)	1.402(7)	1.406	1.390(7)	1.409	1.402(6)	1.402	1.397(4)	1.400(4)	1.406	1.400(3)	1.406
C(8)-N(3)	1.305(8)	1.332	1.320(9)	1.333	1.306(7)	1.326	1.298(4)	1.301(5)	1.327	1.311(3)	1.326
C(8)-C(10)	1.436(10)	1.426	1.425(10)	1.426	1.431(8)	1.377	1.427(5)	1.439(5)	1.430	1.435(4)	1.432
C(10)-C(11)	1.348(9)	1.375	1.338(9)	1.375	1.351(8)	1.377	1.348(5)	1.353(5)	1.377	1.360(4)	1.377
C(11)-O(2)	1.318(8)	1.347	1.350(8)	1.348	1.346(7)	1.350	1.339(4)	1.336(4)	1.344	1.339(3)	1.349
C(8)-C(9)	1.483(9)	1.507	1.497(9)	1.508	1.496(7)	1.510	1.500(5)	1.495(5)	1.511	1.497(4)	1.510

[a] X = O(3) (1-x, -1/2+y, 1/2-z) for **1**, N(1) for **2,** N(4) for **3** and **4** and O(5) for **5**.

[c]In case of B, Mo(2) is involved.

Table S2

X-ray and calculated (DFT/B3LYP methodology) bond angles of complexes **1-5.**

Bond Angles (°)	**1**		**2**		**3**		**4**			**5**	
	obs	calc	obs	Calc	Obs	calc	Obs A	Obs B	calc	obs	calc
O(4)-Mo(1)-O(3)	107.4(2)	106.6	106.8(2)	109.1	106.7(2)	106.6	106.25(12)	105.68(12)	106.3	105.65(10)	105.8
O(3)-Mo(1)-O(2)	99.0(2)	99.7	98.4(2)	99.0	97.5(2)	97.6`	96.55(12)	97.70(12)	96.8	97.35(9)	97.1
O(4)-Mo(1)-O(2)	100.2(2)	100.4	102.2(2)	100.4	104.1(2)	104.1	103.46(11)	105.39(12)	103.0	104.73(8)	103.0
O(3)-Mo(1)-O(1)	100.3(2)	99.8	98.5(2)	97.1	101.2(2)	100.3	97.11(11)	99.0412)	98.5	98.98(9)	100.3
O(4)-Mo(1)-O(1)	96.1(2)	96.9	96.4(2)	100.1	94.7(2)	96.9	96.49(11)	93.83(12)	98.5	94.90(8)	99.2
O(2)-Mo(1)-O(1)	149.7(2)	149.0	150.0(2)	148.0	148.5(2)	147.1	151.54(10)	149.97(11)	148.9	149.95(8)	146.8
O(3)-Mo(1)-N(3)	99.2(2)	104.0	95.2(2)	102.8	92.9(2)	93.6	92.45(11)	93.28(12)	94.0	93.49(9)	94.2
O(4)-Mo(1)-N(3)	152.5(2)	148.8	156.7(2)	147.8	158.2(2)	158.5	159.26(11)	158.11(12)	158.7	158.51(9)	159.3
O(2)-Mo(1)-N(3)	82.3(2)	80.0	81.7(2)	79.7	82.3(2)	79.9	82.73(11)	82.27(11)	80.3	81.90(8)	79.3
O(1)-Mo(1)-N(3)	71.7(2)	71.9	72.2(2)	72.1	71.7(2)	71.7	71.85(10)	72.05(11)	71.7	72.10(7)	71.5
O(3)-Mo(1)-X[a]	174.0(8)	175.3	173.7(2)	180.0	170.3(2)	172.8	170.51(11)	170.95(12)	173.4	171.48(8)	171.8
O(4)-Mo(1)-X[a]	78.4(2)	78.1	79.3(2)	70.9	83.0(2)	80.6	83.13(11)	83.35(12)	80.3	82.87(8)	82.4
O(2)-Mo(1)-X[a]	78.2(2)	78.7	78.7(2)	79.6	80.1(2)	80.1	82.32(10)	79.90(11)	81.2	80.43(7)	80.1
O(1)-Mo(1)-X[a]	80.3(2)	79.9	81.8(2)	79.9	77.2(2)	78.6	80.12(9)	79.66(10)	80.5	79.69(7)	78.7
N(3)-Mo(1)-X[a]	75.2(2)	71.4	79.0(2)	77.3	77.5(2)	79.3	78.06(10)	77.78(11)	79.5	78.08(8)	77.8
C(8)-N(3)-Mo(1)	130.0(4)	129.5	129.0(5)	129.2	127.3(4)	128.0	128.2(3)	128.1(3)	128.4	127.9(2)	127.8
N(2)-N(3)-Mo(1)	116.2(4)	114.6	115.0(4)	114.9	116.2(4)	114.7	115.2(2)	115.5(2)	114.6	115.3(2)	114.6
C(7)-O(1)-Mo(1)	121.8(4)	122.5	119.6(4)	121.7	120.4(4)	122.1	120.6(2)	120.5(2)	122.1	120.2(2)	122.7
C(11)-O(2)-Mo(1)	134.3(4)	139.2	134.6(4)	137.9	129.5(4)	134.7	129.5(2)	131.5(2)	136.3	130.1(2)	134.0
Mo(1)-O(3)-Mo(1)	149.8(2)	159.3	–	–	–	–	–	–	–	–	–
O(2)-C(11)-C(10)	122.4(6)	121.2	122.5(7)	120.9	121.8(5)	121.5	122.9(3)	122.0(4)	121.9	122.7(2)	121.7
C(11)-C(10)-C(8)	128.3(7)	126.0	127.1(7)	125.7	128.6(6)	126.5	127.8(4)	128.2(4)	126.5	126.5(2)	126.4
N(3)-C(8)-C(10)	119.0(6)	122.2	120.6(6)	122.2	119.3(5)	121.8	119.8(3)	119.3(4)	122.1	120.2(2)	121.7
C(8)-N(3)-N(2)	113.8(5)	115.9	116.0(6)	115.8	116.4(5)	117.0	116.6(3)	116.4(3)	116.8	116.8(2)	117.3
C(7)-N(2)-N(3)	109.2(5)	111.7	110.6(5)	111.6	108.2(5)	111.6	110.1(3)	109.5(3)	111.5	109.8(2)	111.2
N(2)-C(7)-O(1)	120.5(5)	118.8	121.7(6)	119.1	123.4(5)	119.7	122.0(3)	122.3(4)	119.8	122.3(2)	120.0

[a] X = O(3) (1-x, -1/2+y, 1/2-z) for **1**, N(1) for **2,** N(4)for **3** and **4** and O(5) for **5**.

Table S3

Geometry of hydrogen-bonding interactions in the crystal structures of the complexes **1**-**5**

D-H	A	H···A (Å)	D···A(Å)	D-H···A(°)	Symmetry code
*Complex **1***					
N(1)-H(1A)	O(2)	2.87(4)	3.72(1)	173(5)	x, 3/2-y, 1/2+z
N(1)-H(1A)	O(4)	2.71(6)	3.30(1)	126(5)	x,3 /2-y, 1/2+z
N(1)-H(1B)	N(2)	1.96(4)	2.701(8)	143	x, y, z
*Complex **2***					
N(1)-H(1A)	O(4)	2.23(2)	3.065(7)	165(7)	x, 1+y, z
N(1)-H(1B)	N(2)	2.15(6)	2.755(8)	127(7)	x, y, z
C(45A)-H(45A)	O(4)	2.73	3.38(2)	125	1-x, 1-y, 1-z
C(43A)-H(43B)	O(4)	2.84	3.54(5)	130	1-x, 1-y, 1-z
C(13)-H(13)	O(41)	2.47	3.20(2)	136	-1+x, y, 1+z
C(9)-H(9B)	O(4)	2.68	3.44(2)	136	-x, 1-y, 1-z
C(3)-H(3)	O(41)	2.50	3.40(2)	164	x, y, 1+z
*Complex **3***					
N(1)-H(1N)	N(2)	2.07(5)	2.717(7)	131(5)	x, y, z
N(1)-H(2N)	O(3)	2.29(2)	3.113(7)	161(6)	-x, y-1/2, 1/2-z
C(9)-H(9B)	O(4)	2.91	3.30(2)	106	x, 1/2-y, 1/2+z
C(4)-H(4)	π	3.42	4.07	129	1-x, -1/2+y, 1/2-z
π	π	4.25	-	-	1-x, -y, 1-z
*Complex **4***					
N(1A)-H(1B)	N(2A)	2.04(3)	2.710(4)	133(4)	x, y, z
N(1A)-H(1A)	O(3A)	2.24(2)	3.076(4)	164(4)	-x, -y, -z
N(1B)-H(1D)	N(2B)	2.13(4)	2.7354(5)	128(4)	x, y, z
N(1B)-H(1C)	O(3B)	2.31(2)	3.146(4)	164(4)	1-x, -y, 1-z
C(20A)-H(20A)	O(4B)	2.42	3.21(1)	143	1-x, 1/2+y, -1/2-z
C(21A)-H(212)	O(4B)	2.50	3.38(1)	151	-x, 1/2+y, -1/2-z
C(15A)-H(15A)	O(4B)	2.82	3.49(1)	130	1-x, -y, 1-z
C(21B)-H(214)	π	2.84	3.73	152	x, ½-y, -1/2+z
*Complex **5***					

N(1)-H(1B)	N(2)	2.05(2)	2.687(3)	131(3)	x,y,z
C(15)-H(15)	O(3)	2.49	3.30(1)	145	1-x, 1/2+y, 1/2-z
C(18)-H(18B)	O(4)	2.49	3.19(1)	129	x,1+y, z
C(9)-H(9C)	O(3)	2.67	3.24(1)	118	1-x, -y, -z
C(19)-H(19C)	O(1)	2.82	3.63(1)	142	x, 1+y, z
C(3)-H(3)	S(1)	3.86	4.77(1)	166	x, 3/2-y, -1/2+z
C(9)-H(9C)	S(1)	3.95	4.30(1)	105	x, y, z
C(19)-H(19C)	O(4)	2.49	3.19(1)	130	-x, 1-y ,-z
π	π	3.96	-	-	1-x, 1/2+y, 1/2-z

Table S4

Energies (a.u.) of the Frontier Orbitals in the complexes **1**-**5**

Complex	HOMO	LUMO
1	-0.2035	-0.1101
2	-0.2098	-0.1119
3	-0.1931	-0.0952
4	-0.1889	-0.0912
5	-0.1937	-0.0913